Electronic Supplementary Information (ESI)

Migratory Insertion of Isocyanide into a Ketenyl-Tungsten Bond as Key Step in Cyclization Reactions

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1. X-ray Crystallography

Single crystals suitable for XRD analysis were selected in Fomblin YR-1800 perfluoropolyether oil (Alfa Aesar) at ambient temperature and mounted on a glass fiber. During the measurement, the samples were cooled to 123(2) or 173(2) K. Diffraction data were collected on a Bruker D8 QUEST diffractometer and a Bruker Kappa Apex II diffractometer using graphite monochromated Mo-K_α radiation. Structure solutions were found by direct methods (SHELXS-97 or SHELXS-2013)[S1] and were refined by full-matrix least-squares procedures on F2 (SHELXL-2013).[S2] All non-hydrogen atoms were anisotropically refined unless stated otherwise. Hydrogen atoms were included at calculated positions with fixed thermal parameters unless stated otherwise. Details of the structure determinations and refinement details for **3**, **4b**, **5**-BF_4, **7-11** are summarized in Tables S1 and S2. Supplementary crystallographic data for this paper can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic details for **3**, **4b**, **5**-BF_4 and **7**.

	3	**4b**	**5**-BF_4	**7**
empirical formula	$C_{23}H_{34}BClN_6O_2W \cdot CH_2Cl_2$	$C_{19}H_{23}BN_6O_3W$	$C_{23}H_{32}BN_6O_3W^+ BF_4^-$	$C_{32}H_{42}BN_7O_4W \cdot 0.84\ CH_2Cl_2$
M_W / g·mol^{-1}	741.60	578.09	722.01	854.72
colour, habit	blue, block	green, block	blue, block	yellow, block
crystal system	triclinic	triclinic	triclinic	triclinic
space group	*P*–1	*P*–1	*P*–1	*P*–1
a / Å	10.2936(4)	9.7834(6)	10.3289(5)	10.2497(9)
b / Å	11.0038(5)	11.1730(7)	11.4973(5)	11.3925(9)
c / Å	13.3415(5)	11.3156(7)	13.0257(6)	16.0476(13)
α / °	98.452(2)	64.197(3)	98.414(1)	105.219(3)
β / °	102.852(2)	72.129(3)	113.051(1)	96.074(3)
γ / °	96.092(2)	88.960(39)	92.169(1)	93.672(3)
V / Å^3	1442.14(10)	1050.19(12)	1400.32(11)	1789.8(3)
Z	2	2	2	2
$\rho_{calcd.}$ / g·cm^{-1}	1.708	1.828	1.712	1.586
μ / mm^{-1}	4.316	5.533	4.187	3.399
$\lambda_{MoK\alpha}$ / Å	0.71073	0.71073	0.71073	0.71073
T / K	123(2)	123(2)	123(2)	173(2)
collected refl.	83572	35050	77362	75962
unique refl.	10022	7562	11395	10418
refl. $I > 2\sigma(I)$	8426	7093	10575	8281
R_{int}	0.1000	0.0427	0.0295	0.1053
parameters/ restraints	348/0	282/1	383/50	461/12

R_1 [$I > 2\sigma(I)$]	0.0462	0.0224	0.0224	0.0429
wR_2 (all data)	0.0987	0.0564	0.0560	0.0837
GooF	1.090	1.074	1.112	1.027
resid. density [eÅ^{-3}]	4.784/–2.446	3.946/–0.700	3.019/–1.350	2.681/–1.458
CCDC	2061110	2061114	2061113	2061111

Table S2. Crystallographic details for **8-11**.

	8	**9**	**10**	**11**
empirical formula	$C_{33}H_{44}BN_7O_4W$ · 0.625 (CH_2Cl_2)	$C_{37}H_{53}BN_8O_3W$	$C_{31}H_{40}BN_7O_4W$ · 1.5 CH_2Cl_2	$C_{62}H_{78}B_2N_{14}O_7W_2$ · 3 CH_2Cl_2
M_W / g·mol^{-1}	850.49	852.53	896.75	1775.48
colour, habit	orange, block	orange, block	yellow, needle	yellow, block
crystal system	monoclinic	monoclinic	triclinic	triclinic
space group	$P2_1/c$	$P2_1/n$	P–1	P–1
a / Å	9.8806(4)	11.4957(14)	9.9415(5)	15.3547(10)
b / Å	22.4324(8)	22.605(3)	11.0539(6)	15.3920(10)
c / Å	17.6641(7)	14.7243(17)	17.5643(9)	17.9913(12)
α / °	90	90	98.146(2)	82.881(2)
β / °	105.658(2)	99.238(2)	97.680(2)	89.831(2)
γ / °	90	90	105.730(2)	62.331(2)
V / Å^3	3769.9(3)	3776.7(8)	1808.92(16)	3729.6(4)
Z	4	4	2	2
$\rho_{calcd.}$ / g·cm^{-1}	1.498	1.499	1.646	1.581
μ / mm^{-1}	3.198	3.105	3.462	3.356
$\lambda_{MoK\alpha}$ / Å	0.71073	0.71073	0.71073	0.71073
T / K	173(2)	173(2)	123(2)	173(2)
collected refl.	111517	106021	86328	214214
unique refl.	13607	15387	12545	21753
refl. $I > 2\sigma(I)$	11878	12752	10776	15024
R_{int}	0.0345	0.0446	0.0585	0.0781
parameters/ restraints	427/0	470/0	412/0	806/0
R_1 [$I > 2\sigma(I)$]	0.0365	0.0241	0.0339	0.0427
wR_2 (all data)	0.0740	0.0570	0.0666	0.0868
GooF	1.242	1.047	1.050	1.070
resid. density [eÅ^{-3}]	2.679/–5.315	1.047/–0.515	2.039/–1.687	2.712/–1.489
CCDC	2061117	2061112	2061116	2061115

2. Molecular structure of 3

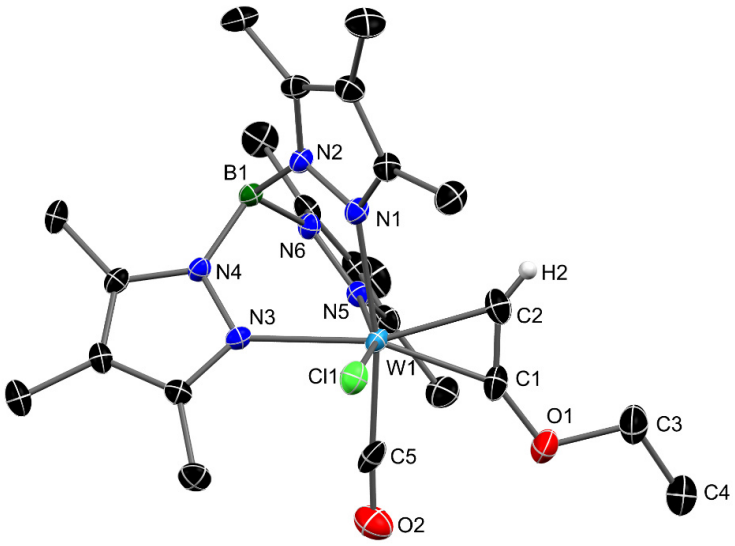


Figure S1. Molecular structure of **3** in the crystal of **3**·1 CH_2Cl_2 with thermal ellipsoids set at 50% probability. Co-crystallized CH_2Cl_2 molecules and Hydrogen atoms except for the alkyne-H have been omitted for clarity. Selected bond lengths [Å]: W1–Cl1 2.4390(11), W1–C1 2.057(5), W1–C2 2.041(5), W1–C5 1.963(5), C1–C2 1.274(7), C1–O1 1.320(6).

3. Molecular structure of 4a

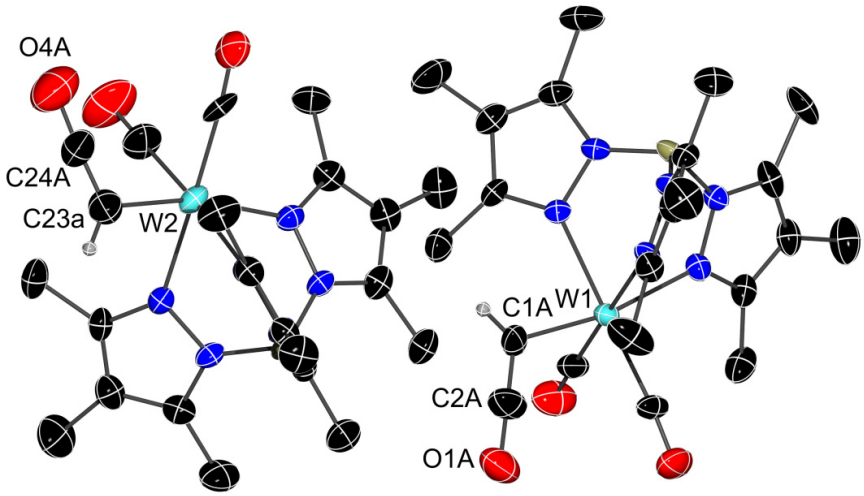


Figure S2. Molecular structure of **4a** in the crystal of **4a** · 0.75 CH_2Cl_2 with thermal ellipsoids set at 50 % probability . Co-crystallized CH_2Cl_2 molecules and hydrogen atoms except for the ketenyl-H have been omitted for clarity. Both individual complex molecules with the major occupation for the disordered CO/HCCO ligands are shown. The data quality solely allows a proof of identity.

4. Molecular structure of 5-BF_4

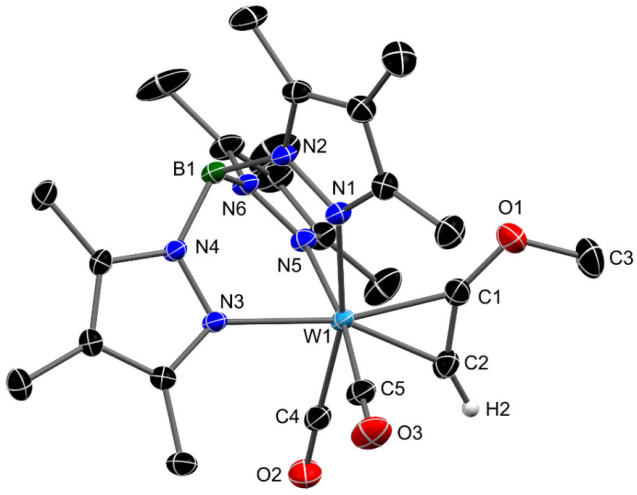


Figure S3. Molecular structure of $\mathbf{5}^+$ in the crystal of **5**-BF_4 with thermal ellipsoids set at 50% probability. Hydrogen atoms except for the alkyne-H and anions have been omitted for clarity. Selected bond lengths [Å]: W1–C1 2.000(2), W1–C2 2.028(2), W1–C4 2.019(2), W1–C5 2.066(2), C1–C2 1.339(3), C1–O1 1.300(3).

5. Molecular structure of 6

Due to mosaicity of the crystals and resulting large residual electron density only the overall structural identity of **6** can be derived. Some parameters are given: cell 15.4726, 11.6809, 32.1040, 90.000, 96.247, 90.000; R1 = 0.0328 for 17489 reflexes $F_o > 4\sigma(F_o)$; R1 = 0.0452 for all 20868 detected reflexes; highest difference peak 2.341, deepest hole –3.321.

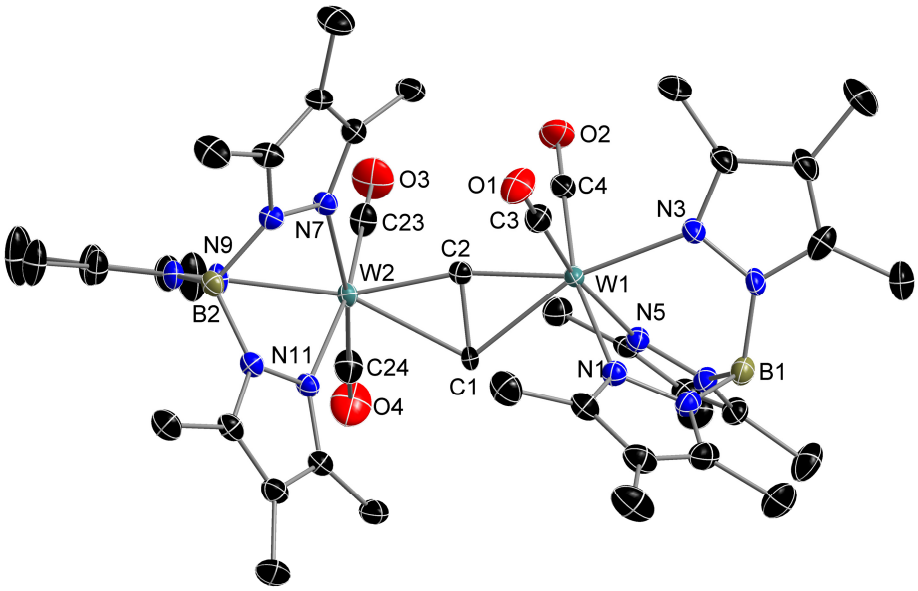


Figure S4. Molecular structure of **6** in the crystal of **6**·toluene with thermal ellipsoids set at 50% probability. Hydrogen atoms and solvents molecules have been omitted for clarity. Selected bond lengths [Å]: W1–C1 2.305(2), W1–C2 1.968(2), W2–C1 2.360(2), W2–C2 1.991(2).

6. Molecular structure of 7

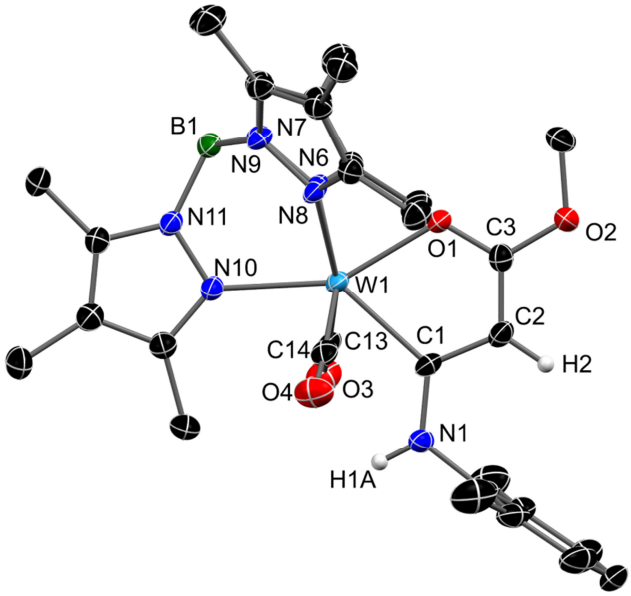


Figure S5. Molecular structure of **7** in the crystal with thermal ellipsoids set at 50% probability. Hydrogen atoms except for H1A and H2 have been omitted for clarity. Selected bond lengths [Å]: W1–C1 2.183(4), W1–O1 2.115(3), C1–C2 1.399(6), C1–N1 1.357(5), C2–C3 1.367(4), C3–O1 1.272(5), C3–O2 1.349(5).

7. Molecular Structure of 9

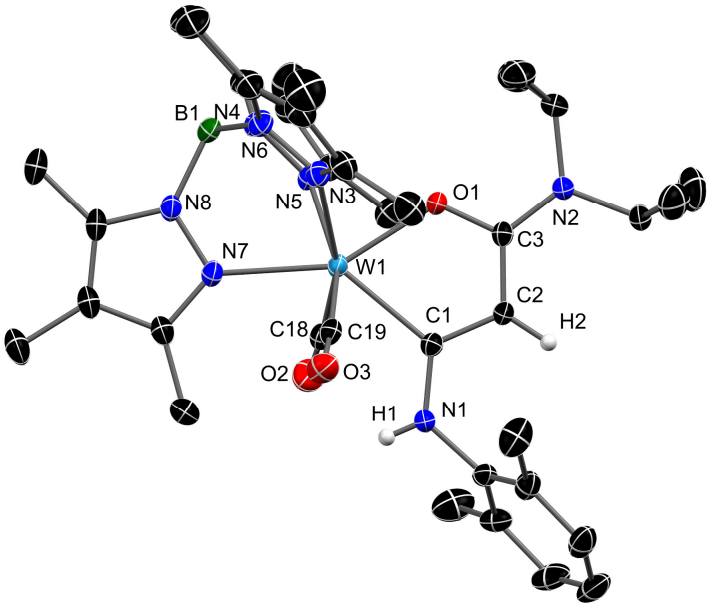


Figure S6. Molecular structure of **9** in the crystal with thermal ellipsoids set at 50% probability. Hydrogen atoms except for H1 and H2 have been omitted for clarity. Selected bond lengths [Å]: W1–C1 2.1707(16), W1–O1 2.0845(12), C1–C2 1.388(2), C1–N1 1.369(2), C2–C3 1.401(2), C3–O1 1.290(2), C3–N2 1.359(2).

8. Cyclic voltammetry

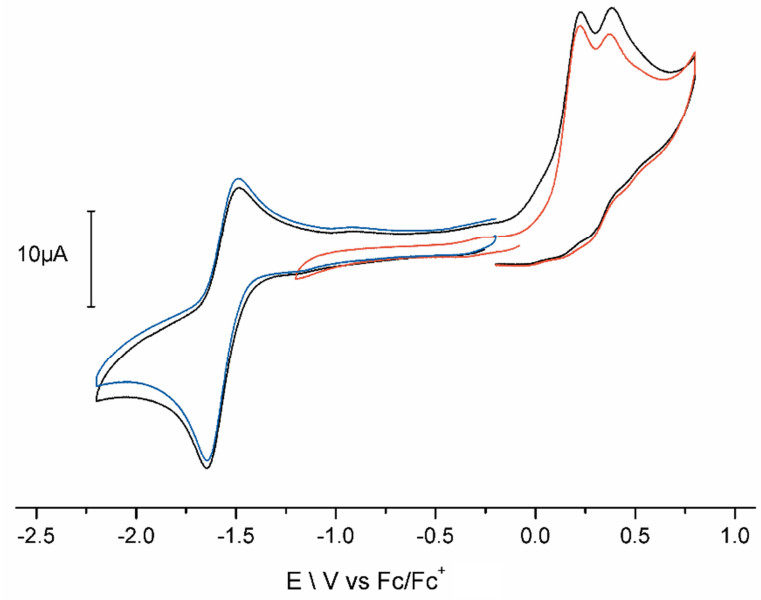


Figure S7. Cyclic voltammetry of compound **4a** in 0.1 M *n*-Bu_4NPF_6/CH_2Cl_2 solution with different scanning width.

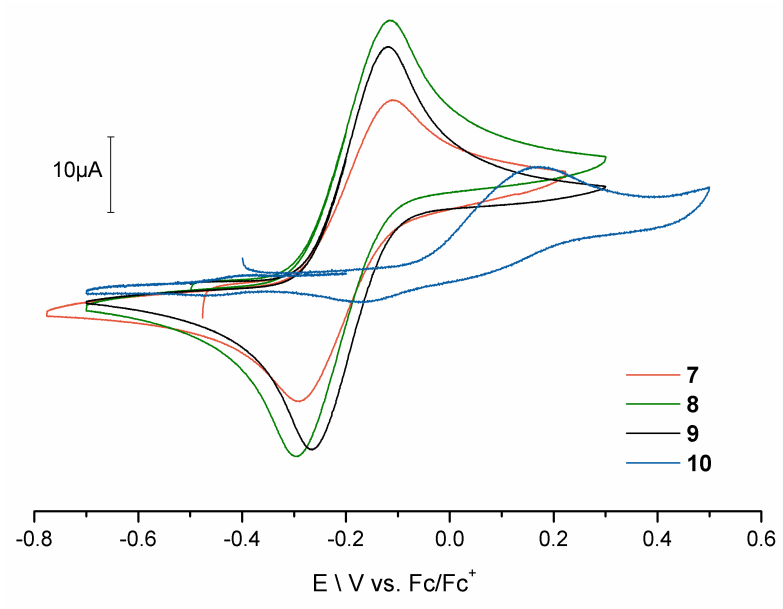


Figure S8. Selected cyclic voltammetry of the oxametallacycles **7** to **10** in a 0.1 M *n*-Bu_4NPF_6/CH_2Cl_2 solution.

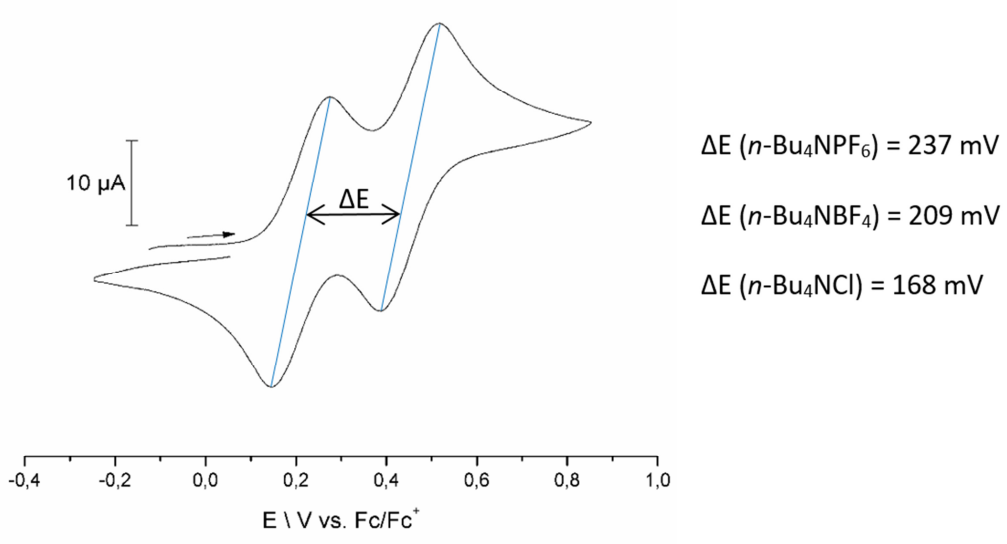


Figure S9. Cyclic voltammetry of **11** with the difference between the reversible redox potentials in different conducting salt solutions (0.1 M in CH_2Cl_2).

9. Spectroelectrochemistry of 11

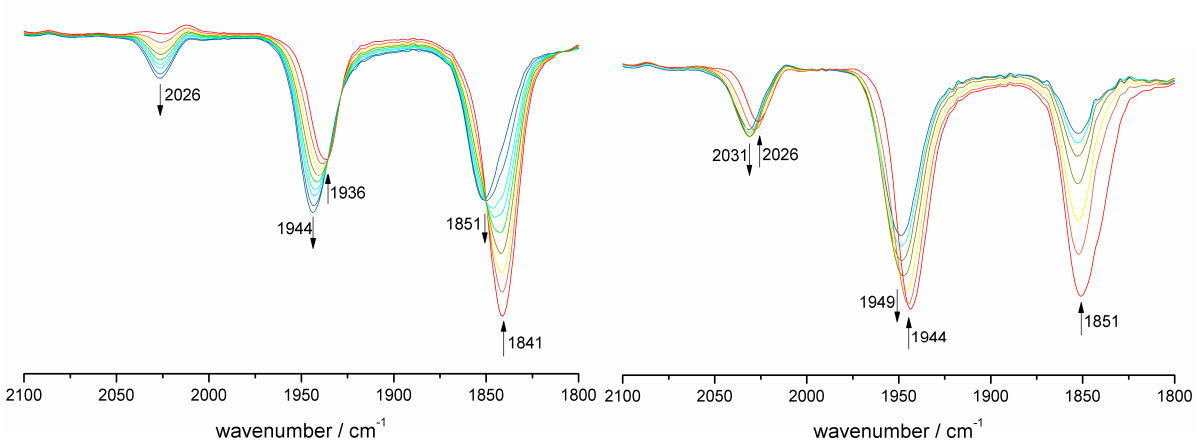


Figure S10. Selected IR spectra in DCE solution of **11** at the redox potentials 0.21 V (left, **11** (red) to **11**$^{+}$ (blue)) and 0.45 V (right, **11**$^{+}$ (red) to **11**$^{2+}$ (blue)) over time.

Calculations of the charge delocalization of W^{III} on the W^{II} center in the mixed-valent complex **11**$^{+}$ {Δp_1 for the lower CO band (1841 cm^{-1}) and Δp_2 for the higher CO band (1936 cm^{-1})}**.**

$$\Delta p = \frac{(\Delta\tilde{\nu}_{ox} + \Delta\tilde{\nu}_{red})}{2(\tilde{\nu}'_{ox} - \tilde{\nu}'_{red})}$$

$$\Delta p_1 = \frac{(5+10)}{2(1949-1841)} = 0.069 \qquad \Delta p_2 = \frac{(5+8)}{2(2031-1936)} = 0.068$$

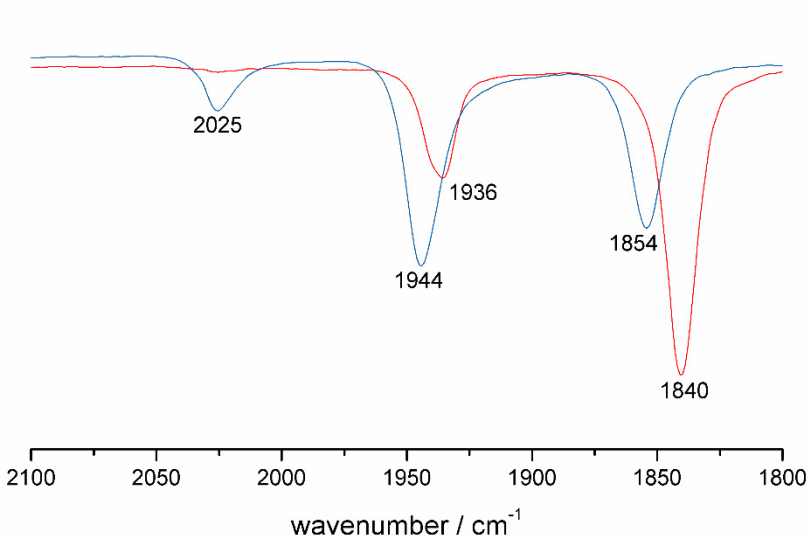


Figure S11. Selected IR spectra in THF solution of **11** (red) and **11**$^{+}$ (blue) after stoichiometric oxidation with [Fc]PF_6.

10. NMR spectra

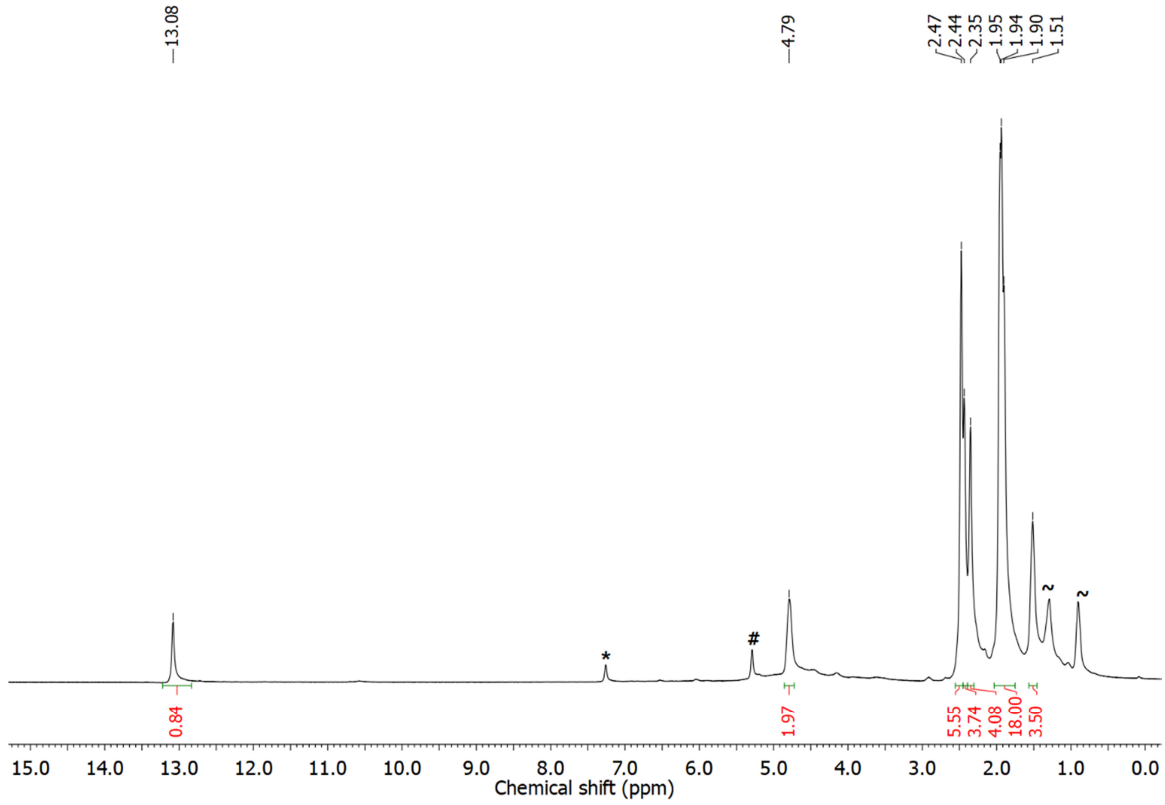


Figure S12. ^{1}H NMR spectrum of **2a**-PF_6 in $CDCl_3$ (*), # CH_2Cl_2, ~ *n*-pentane.

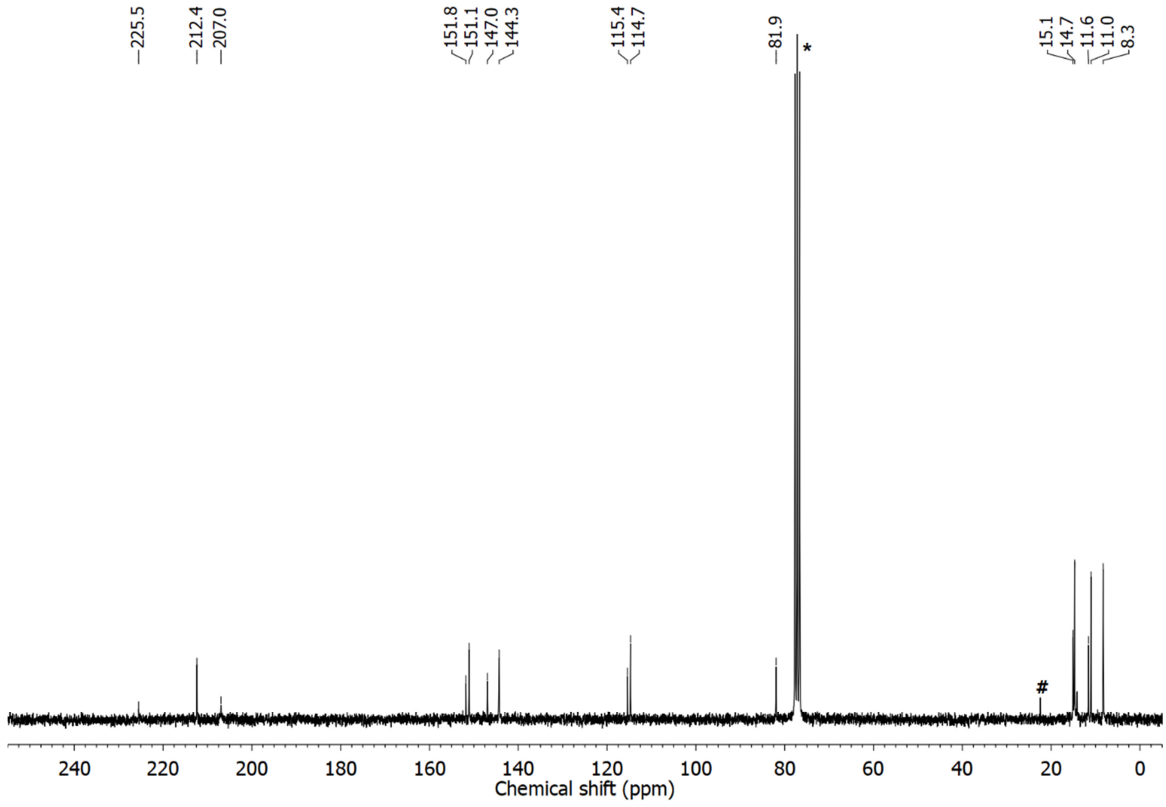


Figure S13. ^{13}C NMR spectrum of **2a**-PF_6 in $CDCl_3$ (*), # *n*-pentane.

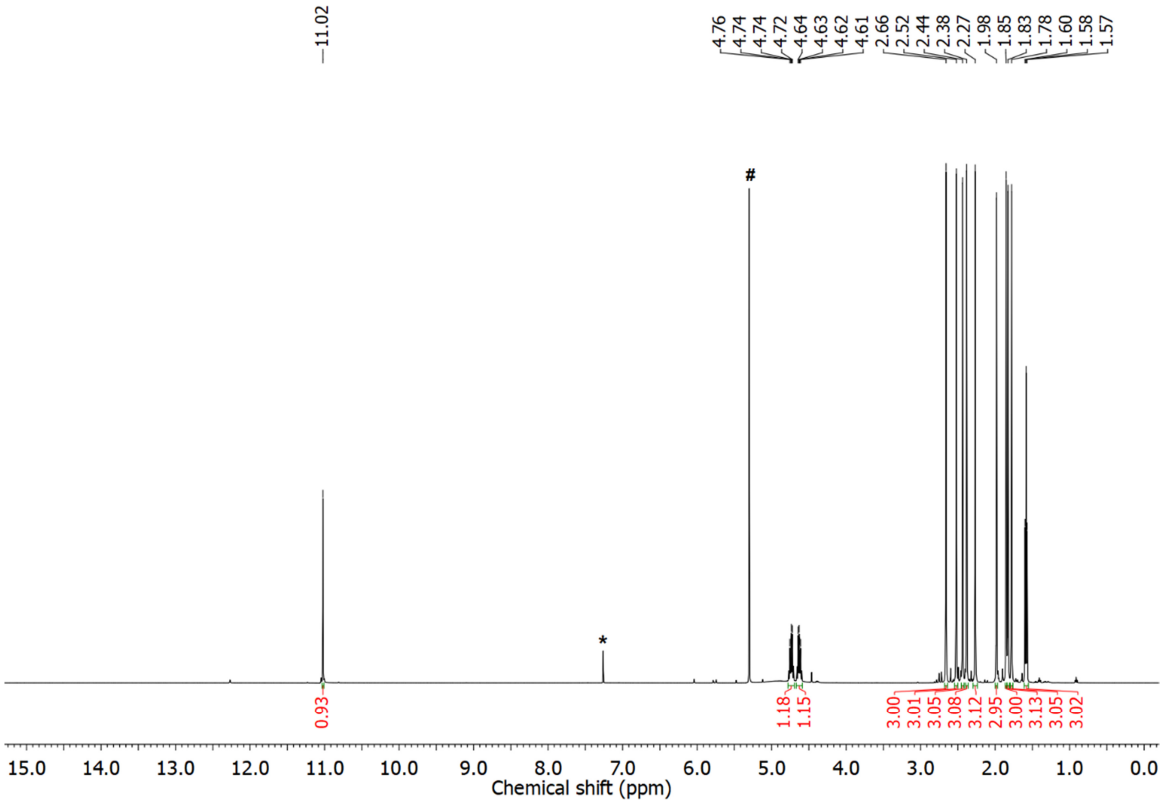


Figure S14. ^{1}H NMR spectrum of **3** in $CDCl_3$ (*), # CH_2Cl_2.

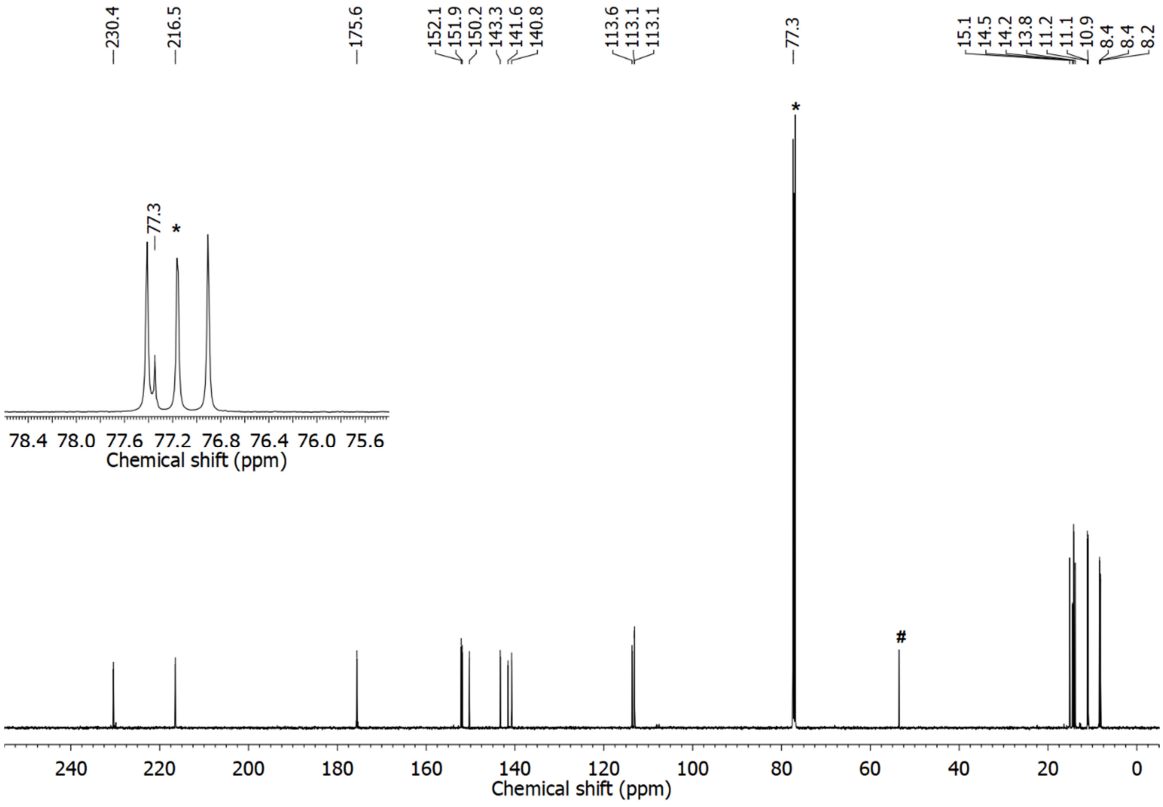


Figure S15. ^{13}C NMR spectrum of **3** in $CDCl_3$ (*), # CH_2Cl_2.

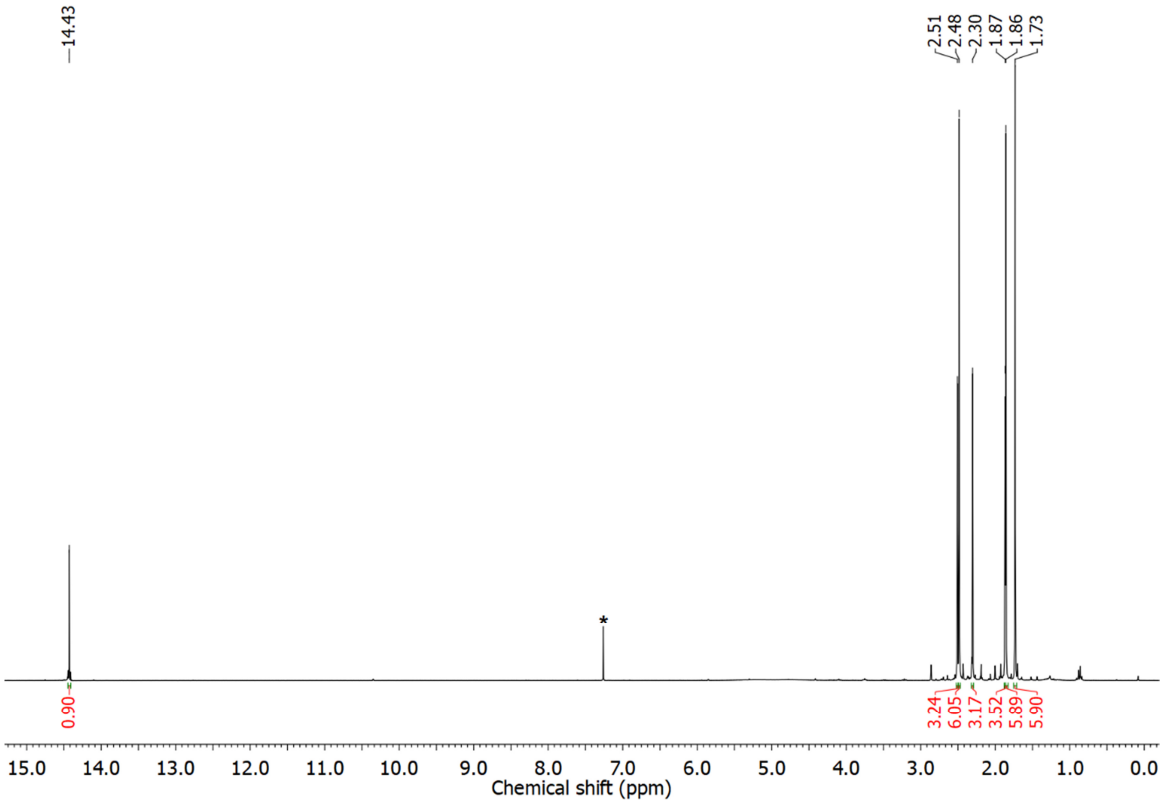


Figure S16. ^{1}H NMR spectrum of **4a** in $CDCl_3$ (*).

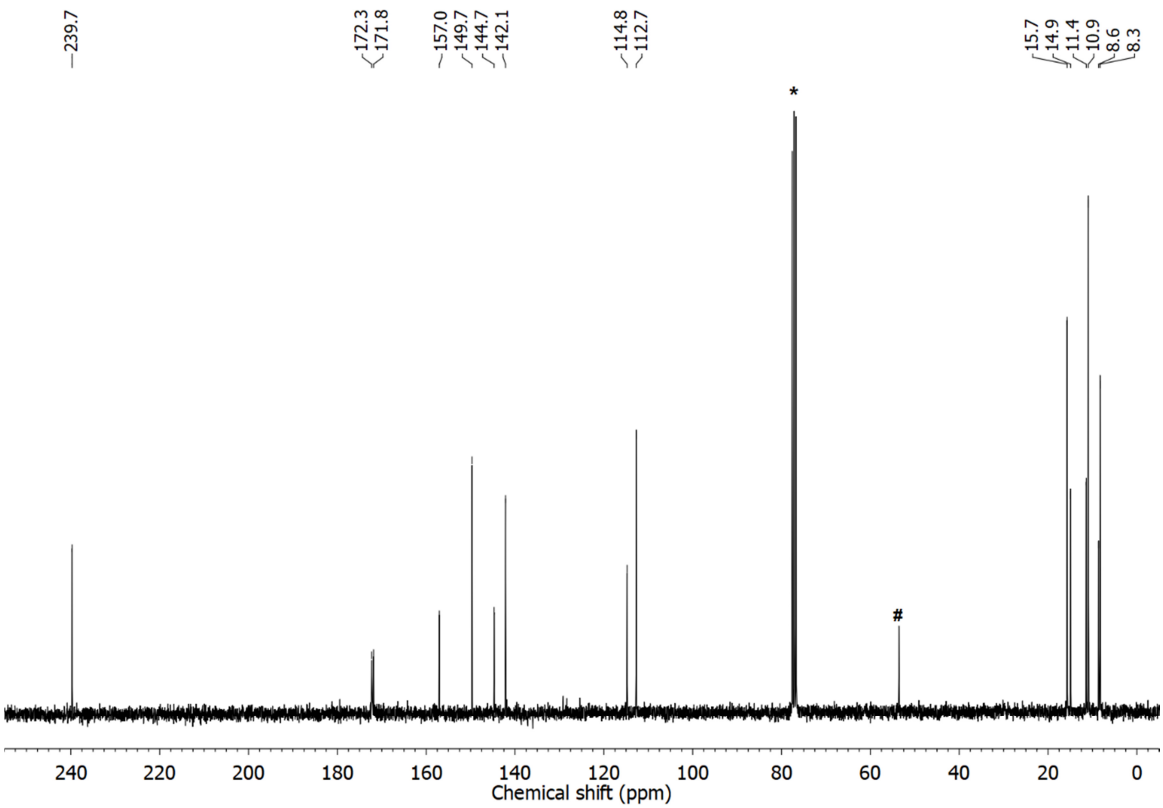


Figure S17. ^{13}C NMR spectrum of **4a** in $CDCl_3$ (*), # CH_2Cl_2.

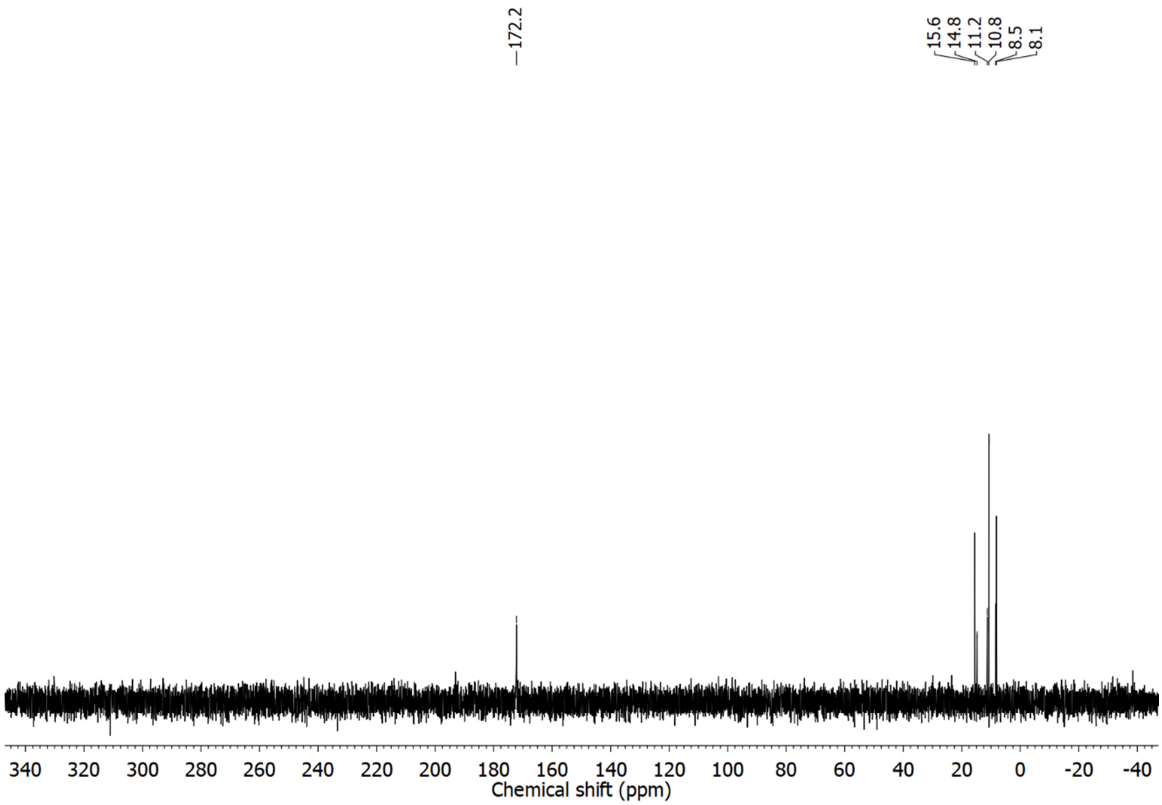


Figure S18. ^{13}C DEPT spectrum NMR of **4a** in $CDCl_3$.

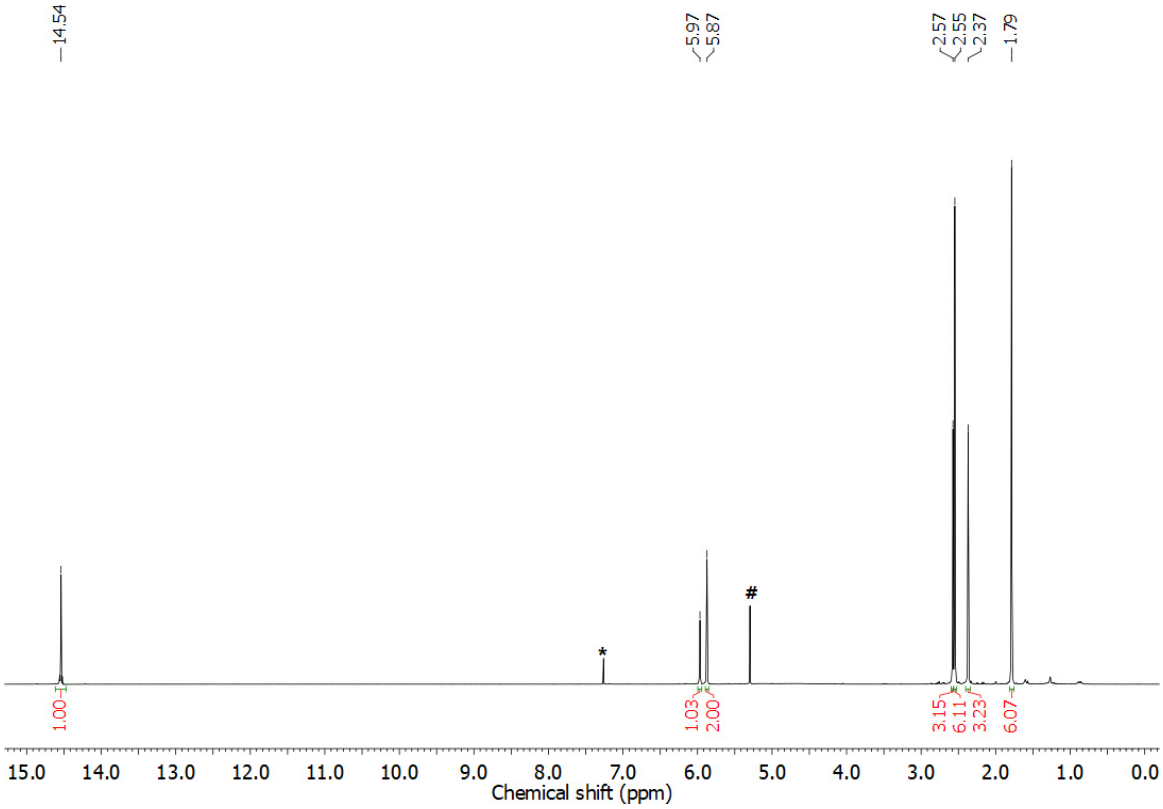


Figure S19. ^{1}H NMR spectrum of **4b** in $CDCl_3$ (*), # CH_2Cl_2.

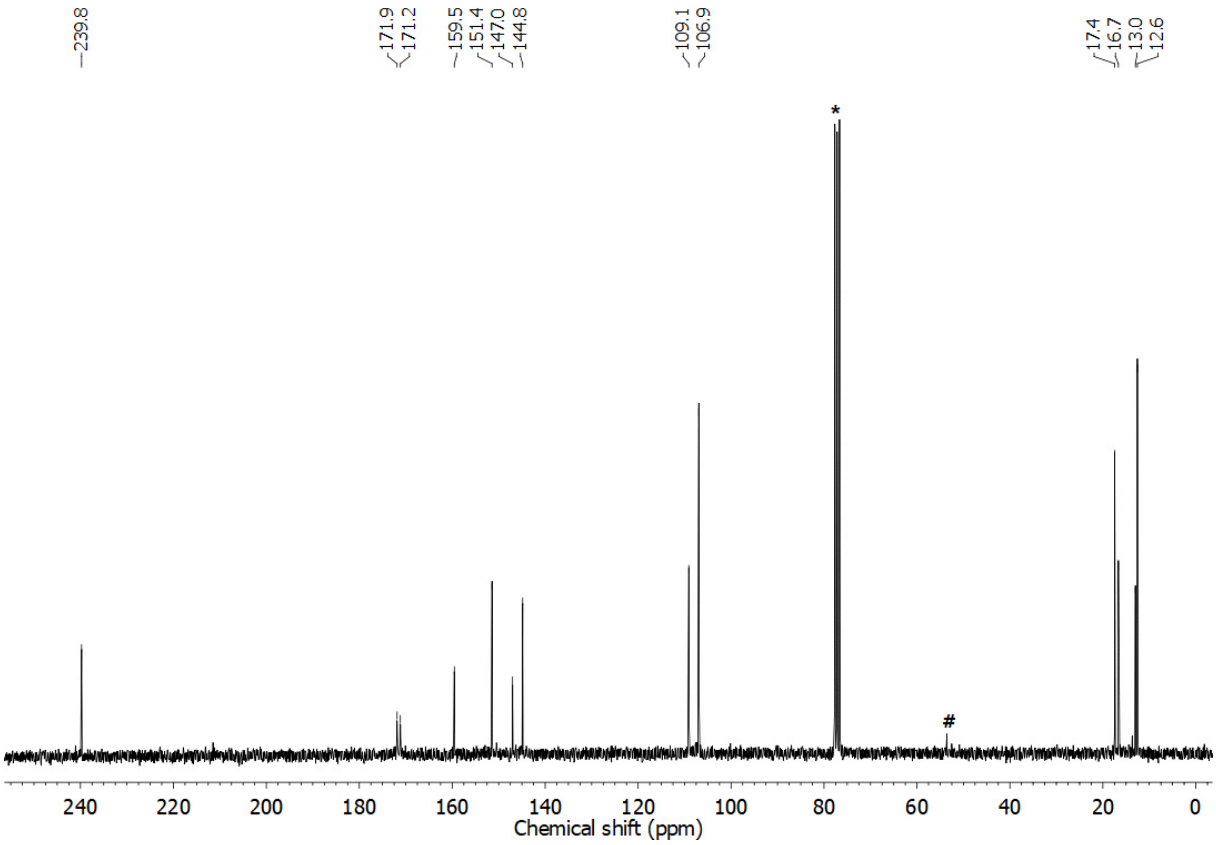


Figure S20. ^{13}C NMR spectrum of **4b** in $CDCl_3$ (*), # CH_2Cl_2.

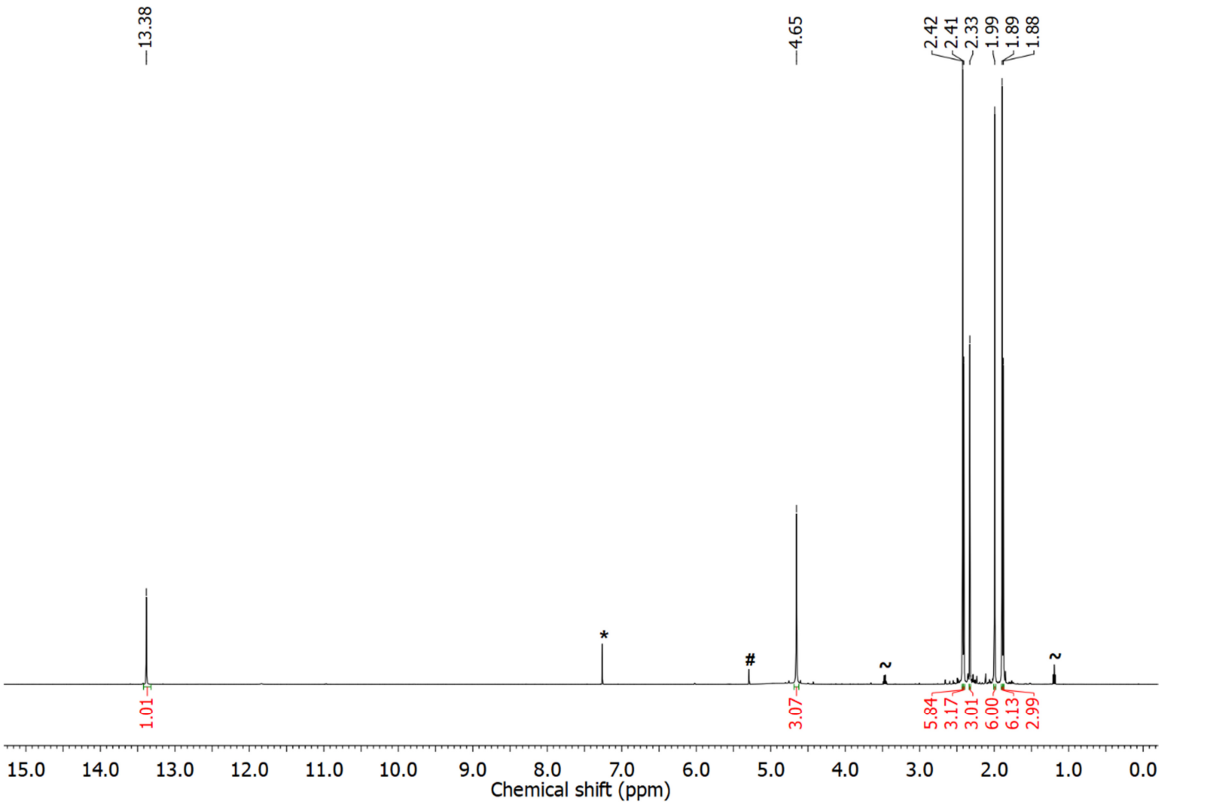


Figure S21. ^{1}H NMR spectrum of **5** in $CDCl_3$ (*), # CH_2Cl_2, ~ diethyl ether.

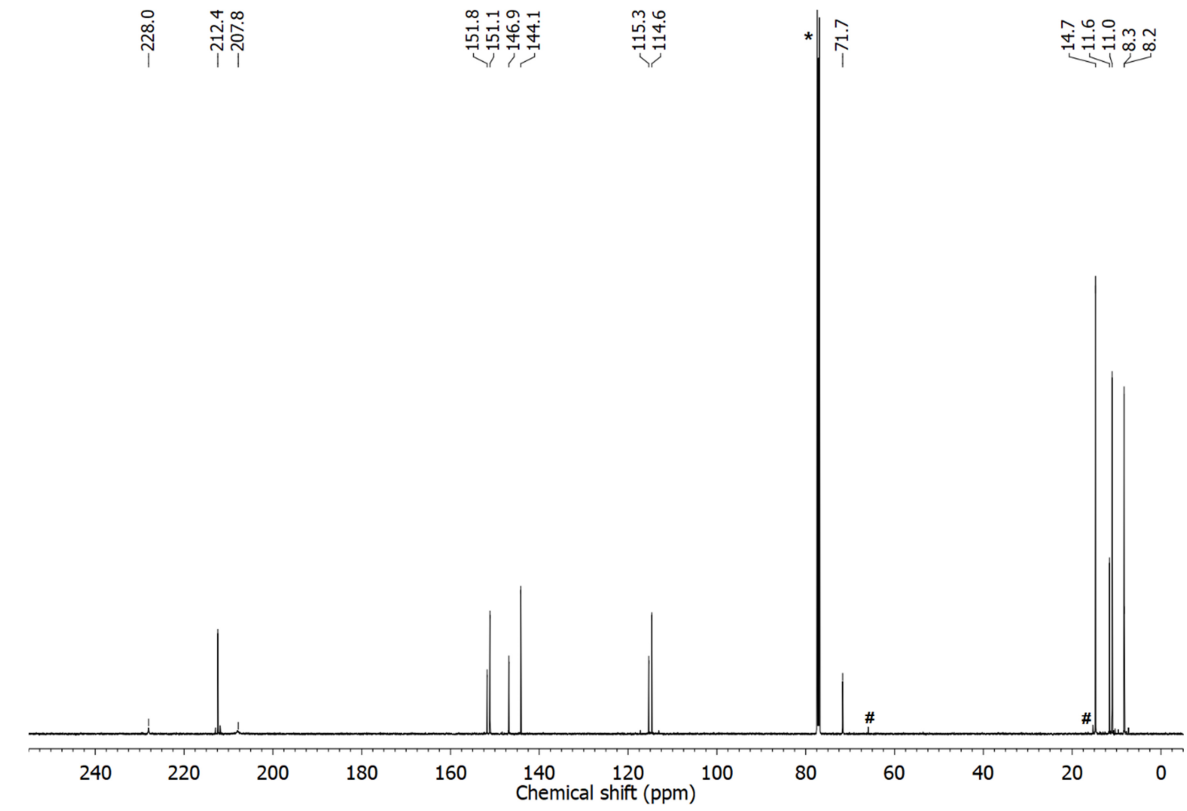


Figure S22. ^{13}C NMR spectrum of **5** in $CDCl_3$ (*), # diethyl ether.

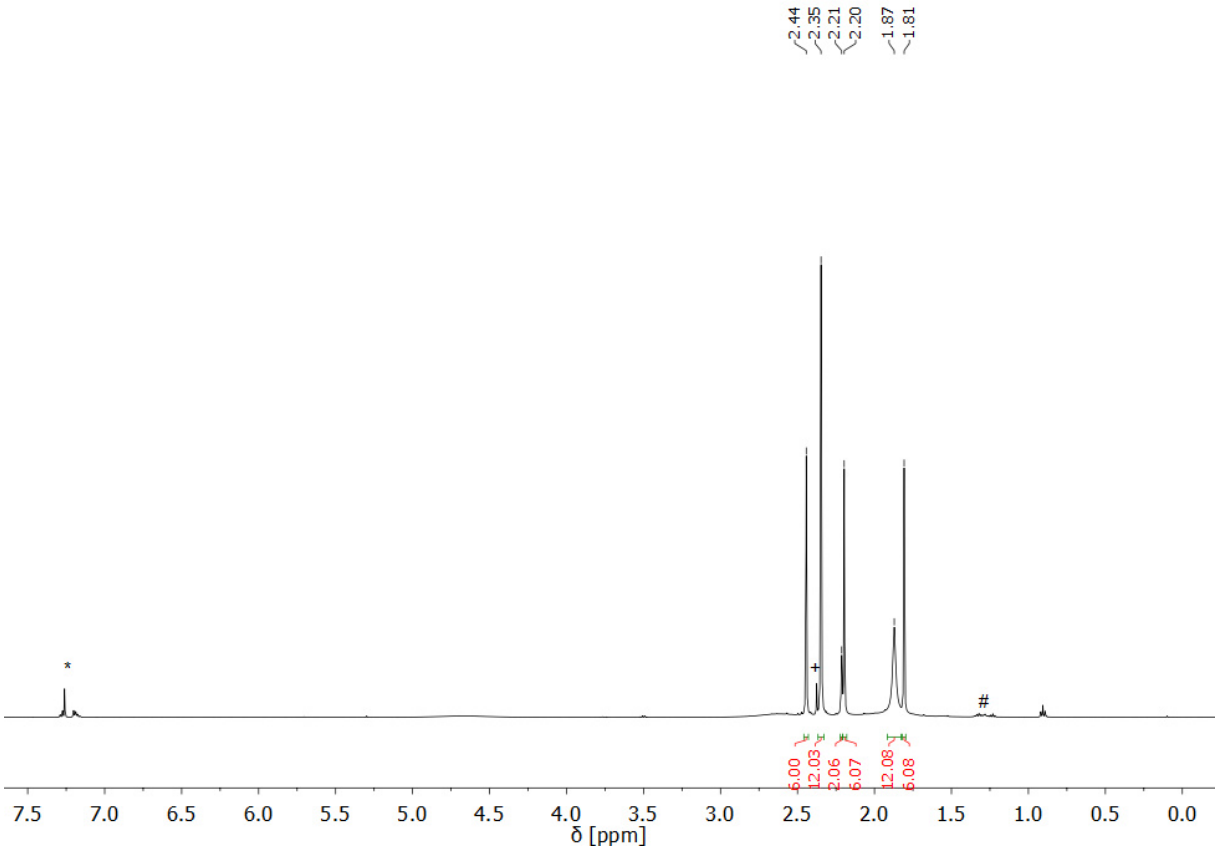


Figure S23. ^{1}H NMR spectrum of **6** in $CDCl_3$ (*) at 298.2 K, # *n*-pentane, + toluene .

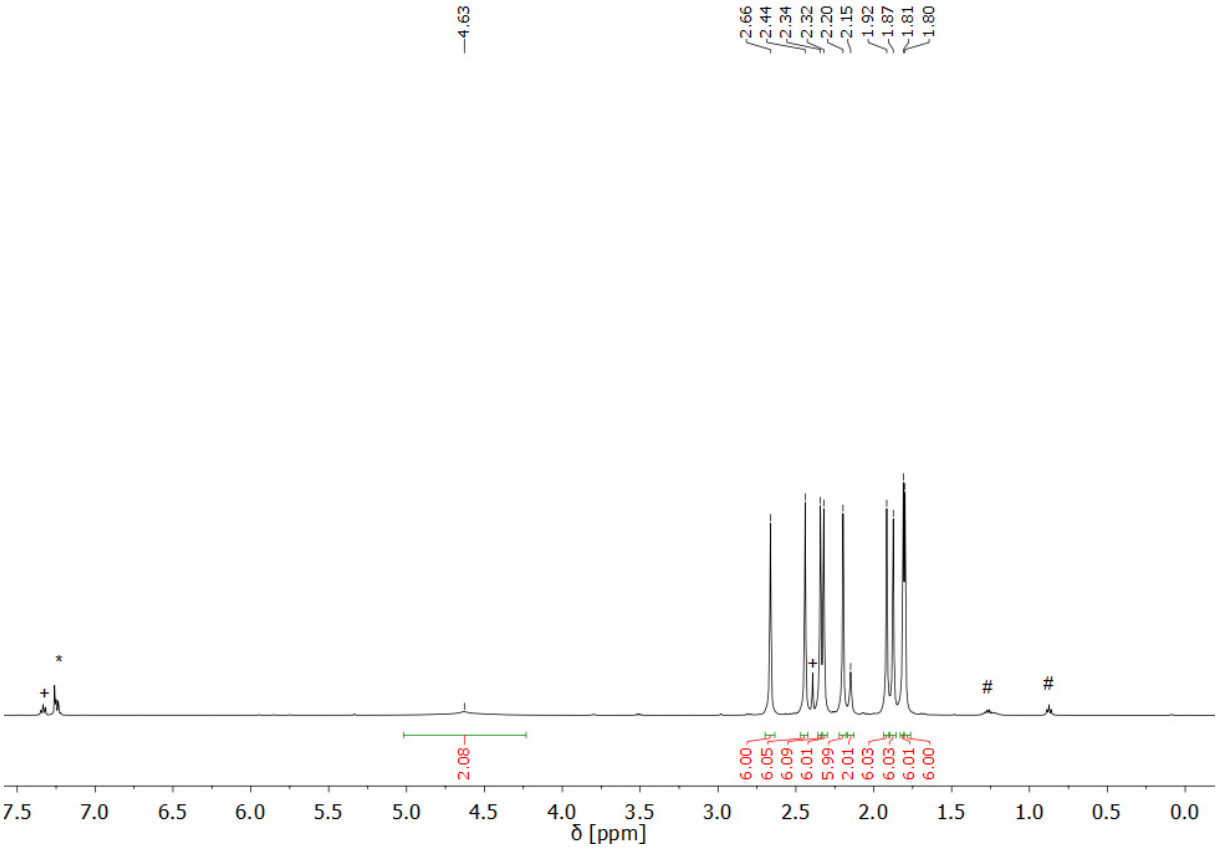


Figure S24. ^{1}H NMR spectrum of **6** in $CDCl_3$ (*) at 195.2 K, # *n*-pentane, + toluene .

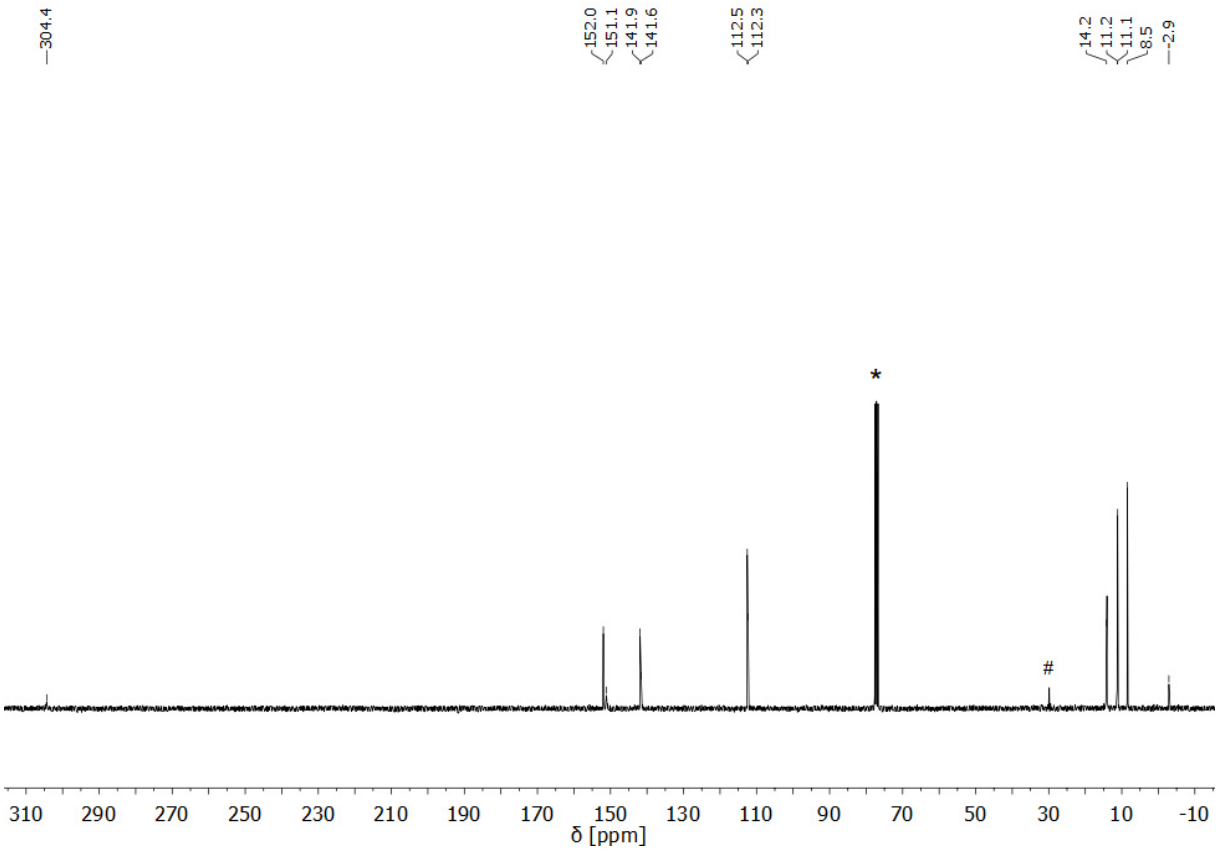


Figure S25. ^{13}C NMR spectrum of **6** in $CDCl_3$ (*), # *n*-pentane .

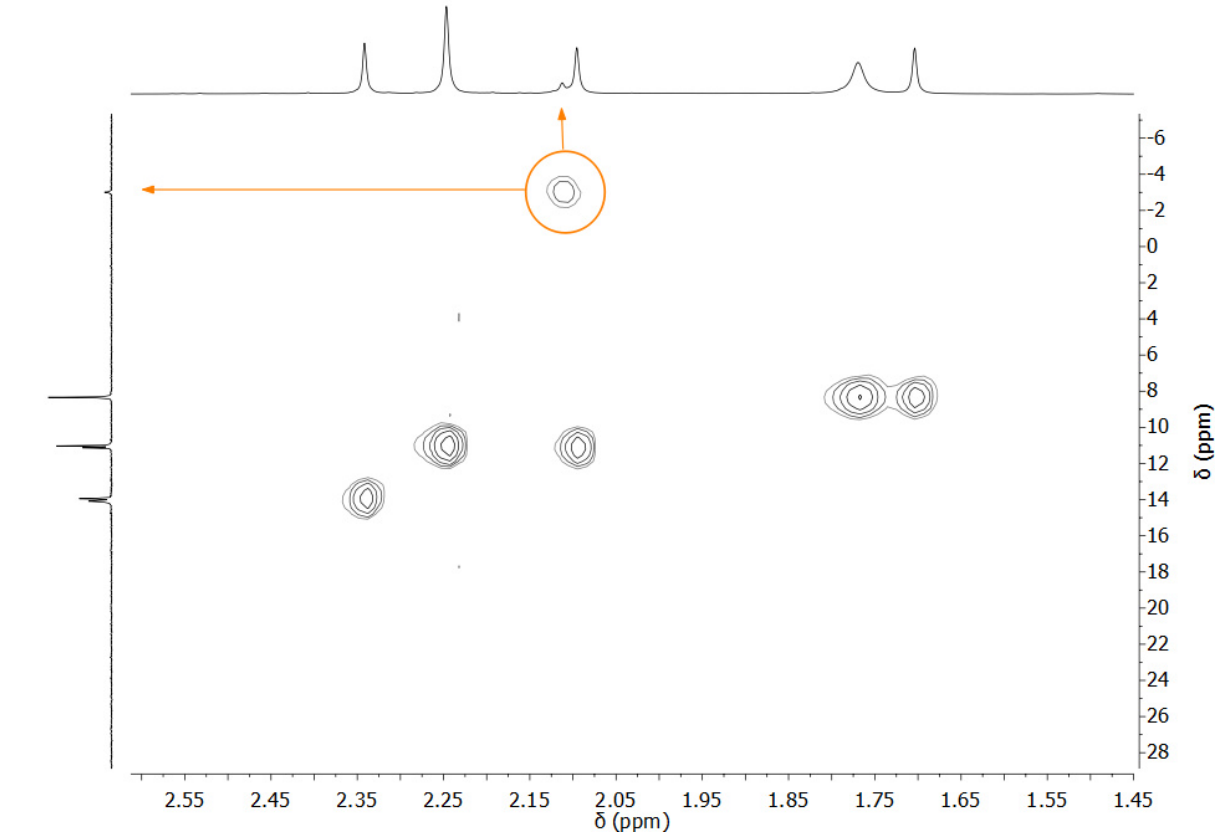


Figure S26. $^{1}H^{13}C$ HSQC NMR spectrum of **6** in $CDCl_3$.

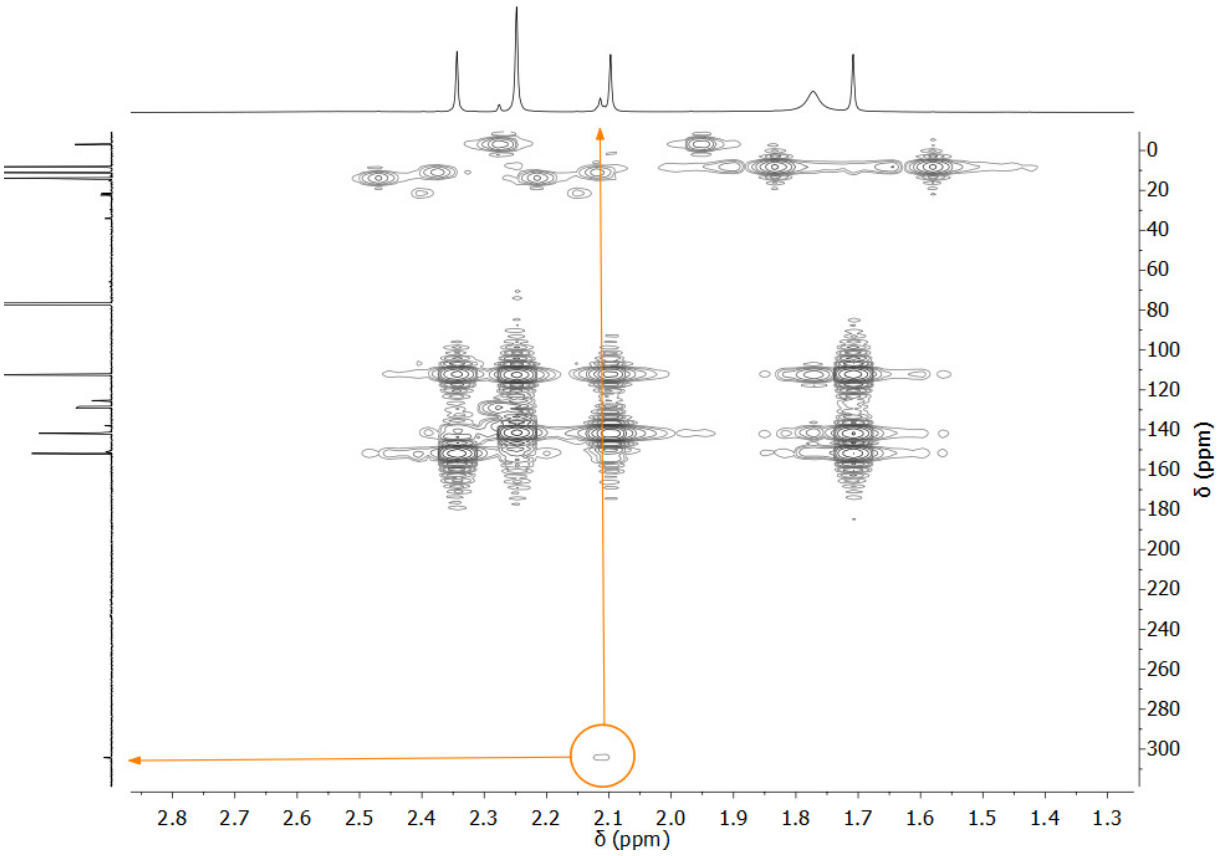


Figure S27. $^{1}H^{13}C$ HMBC NMR spectrum of **6** in $CDCl_3$.

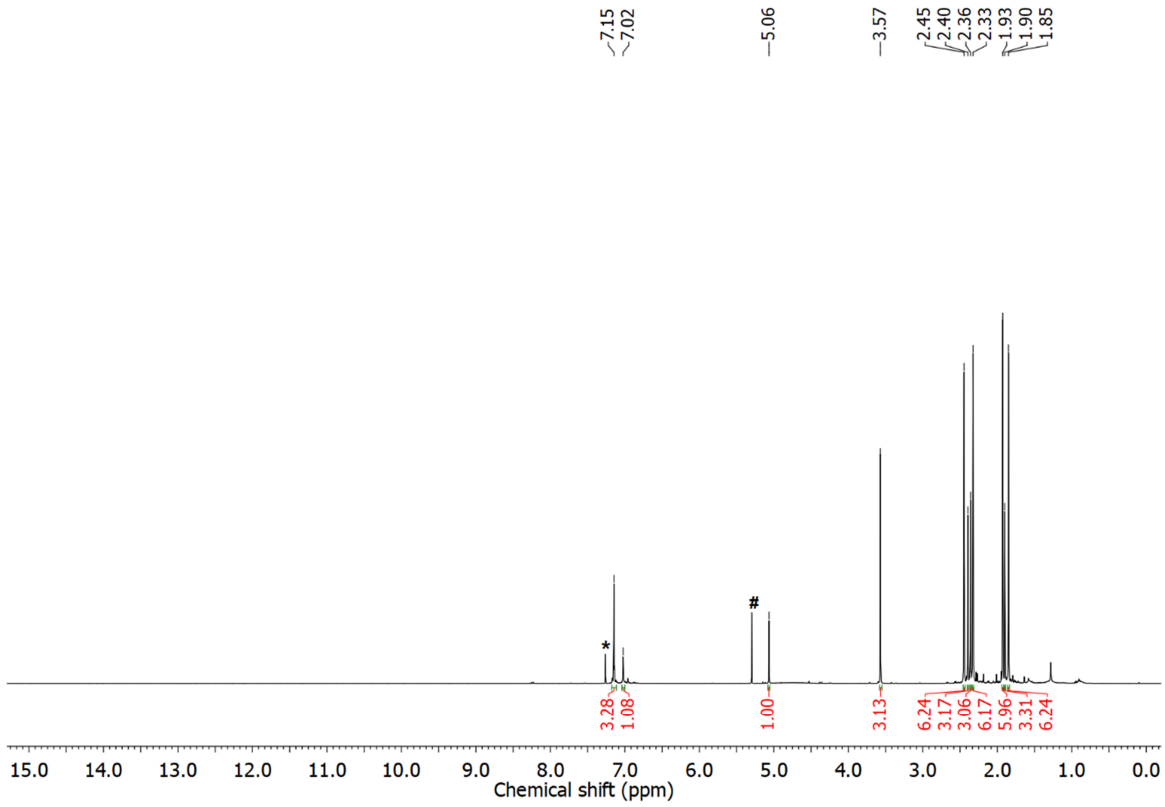


Figure S28. ^{1}H NMR spectrum of **7** in $CDCl_3$ (*), # CH_2Cl_2.

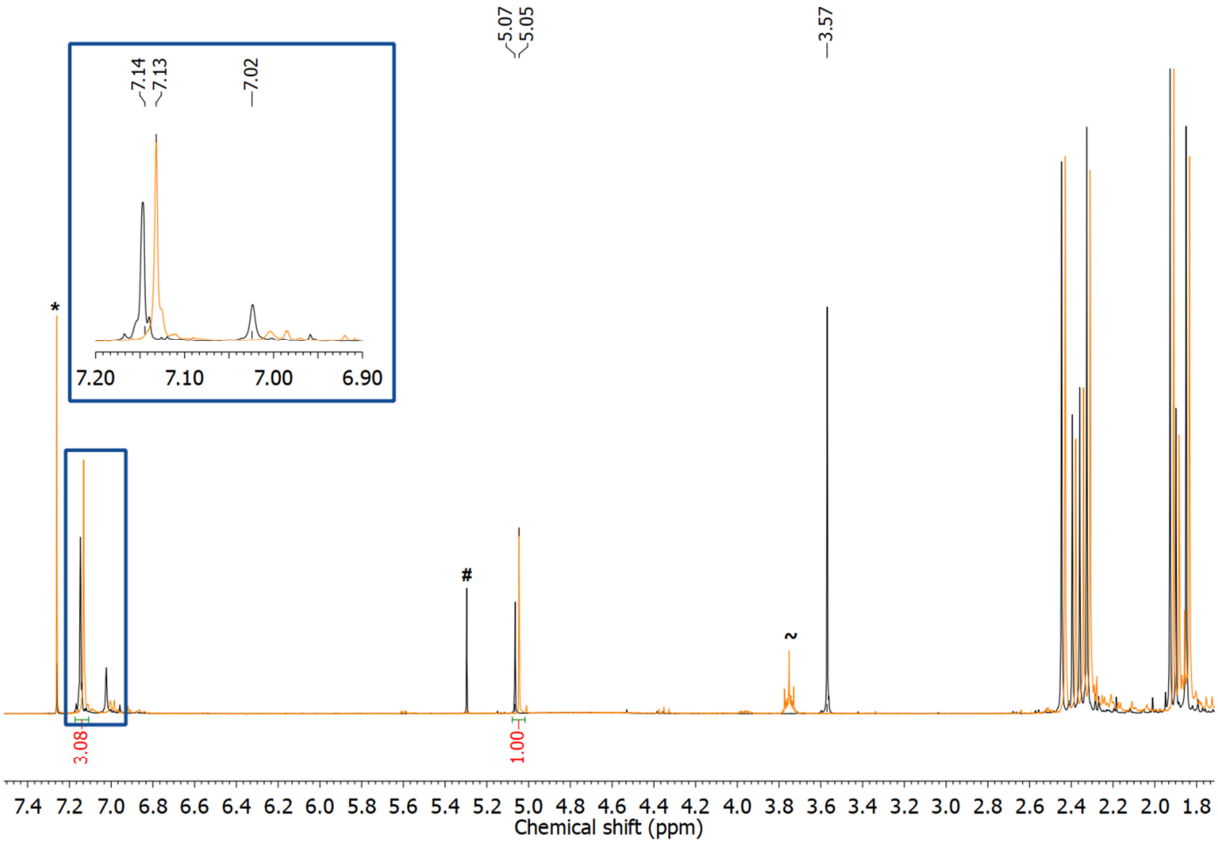


Figure S29. ^{1}H NMR spectrum of **7** (black) and **7** prepared with CD_3OD (red) in $CDCl_3$; $CHCl_3$ (*), # CH_2Cl_2, ~THF.

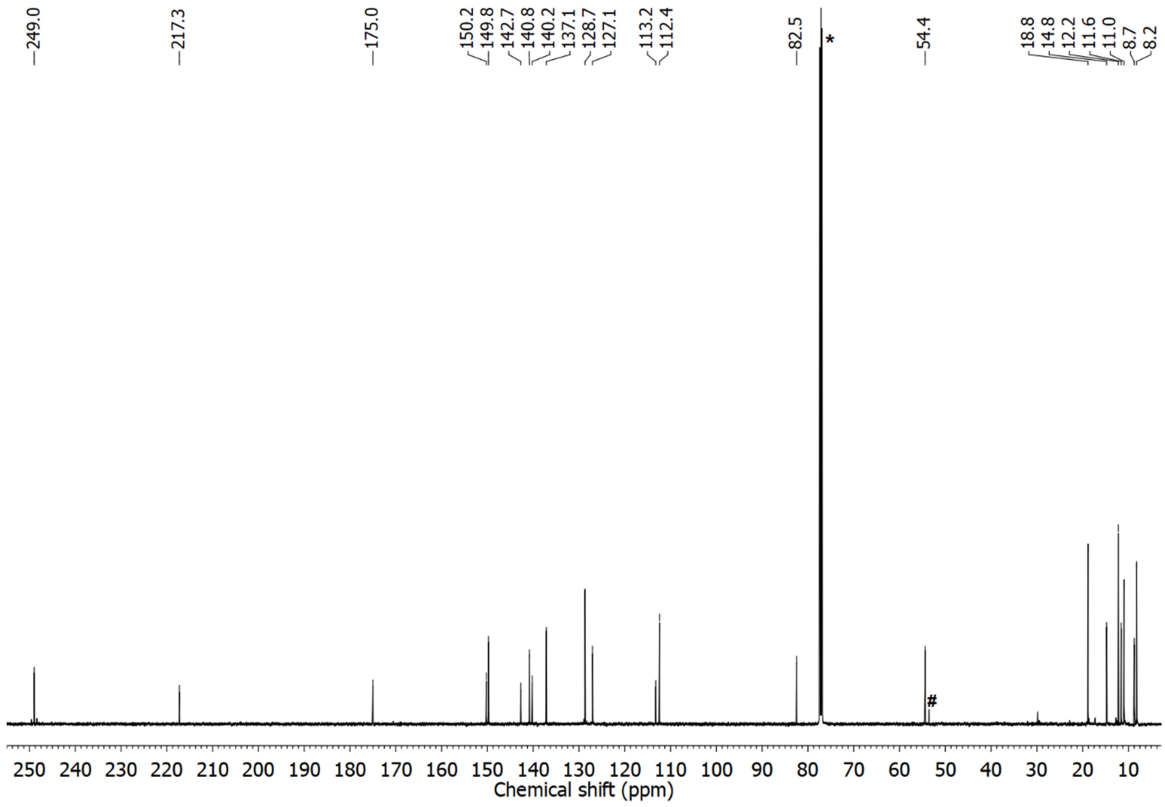


Figure S30. ^{13}C NMR spectrum of **7** in $CDCl_3$ (*), # CH_2Cl_2.

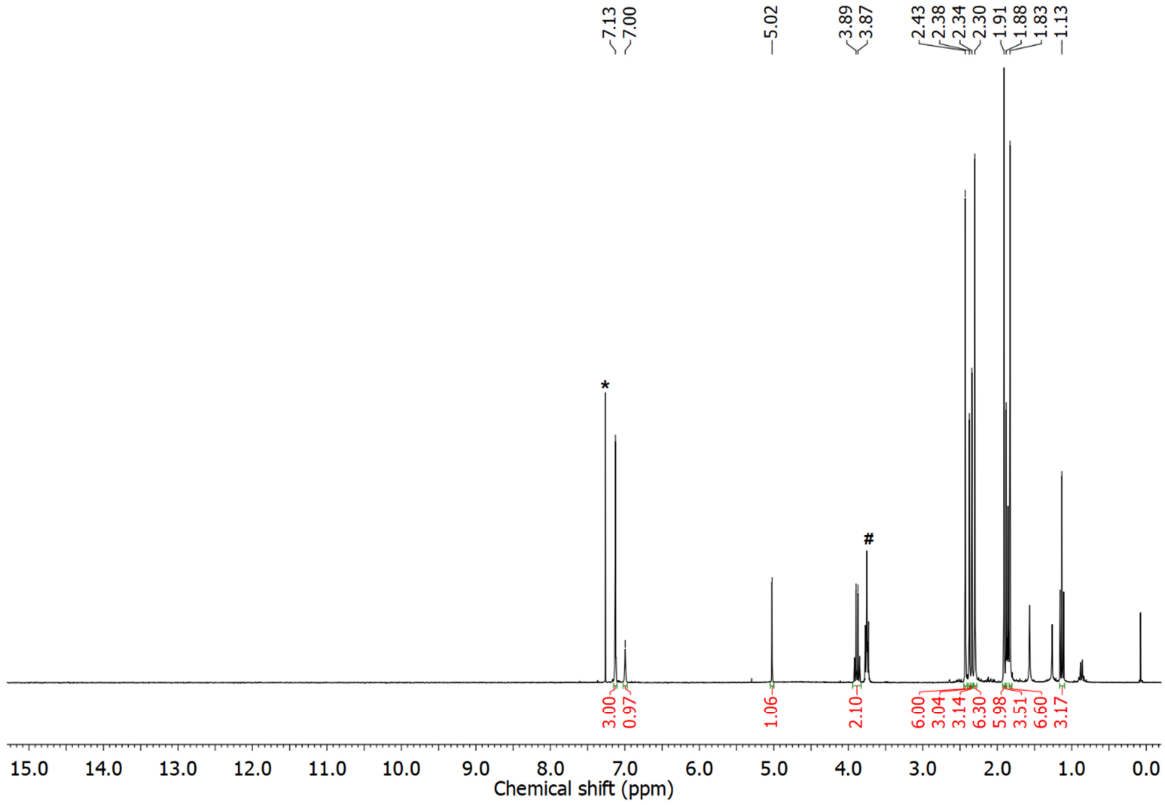


Figure S31. ^{1}H NMR spectrum of **8** in $CDCl_3$ (*), # THF.

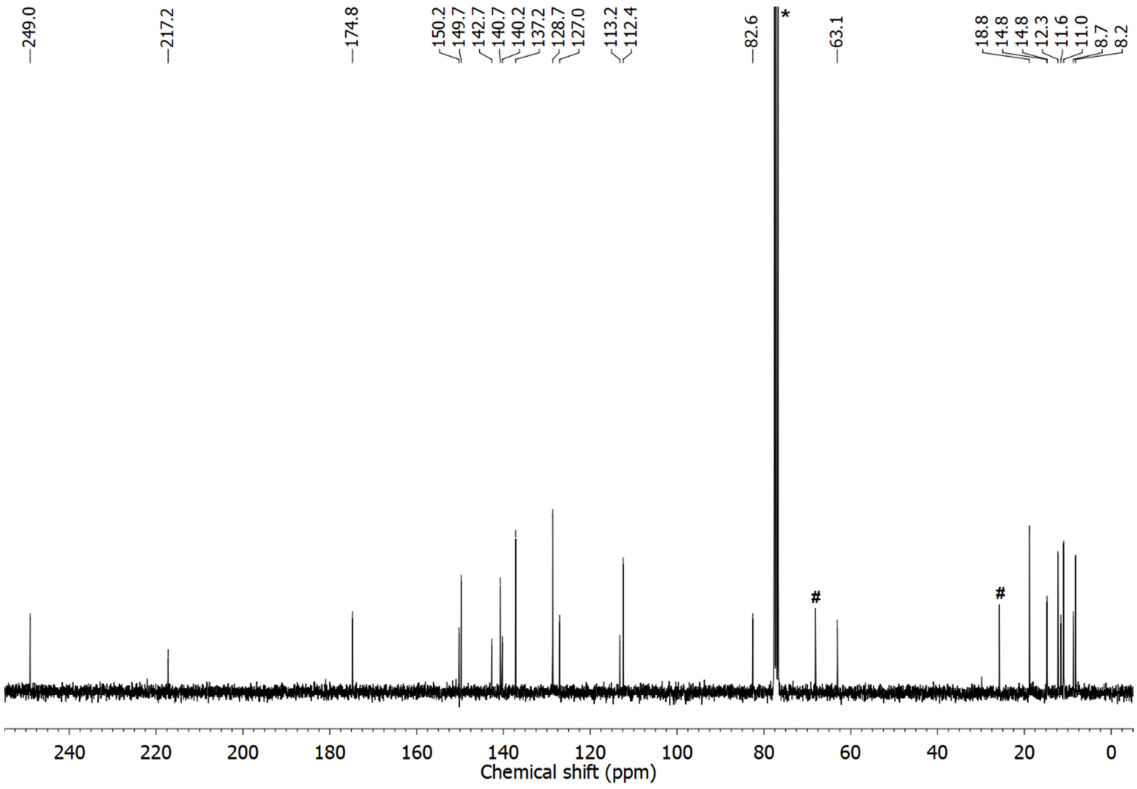


Figure S32. ^{13}C NMR spectrum of **8** in $CDCl_3$ (*), # THF.

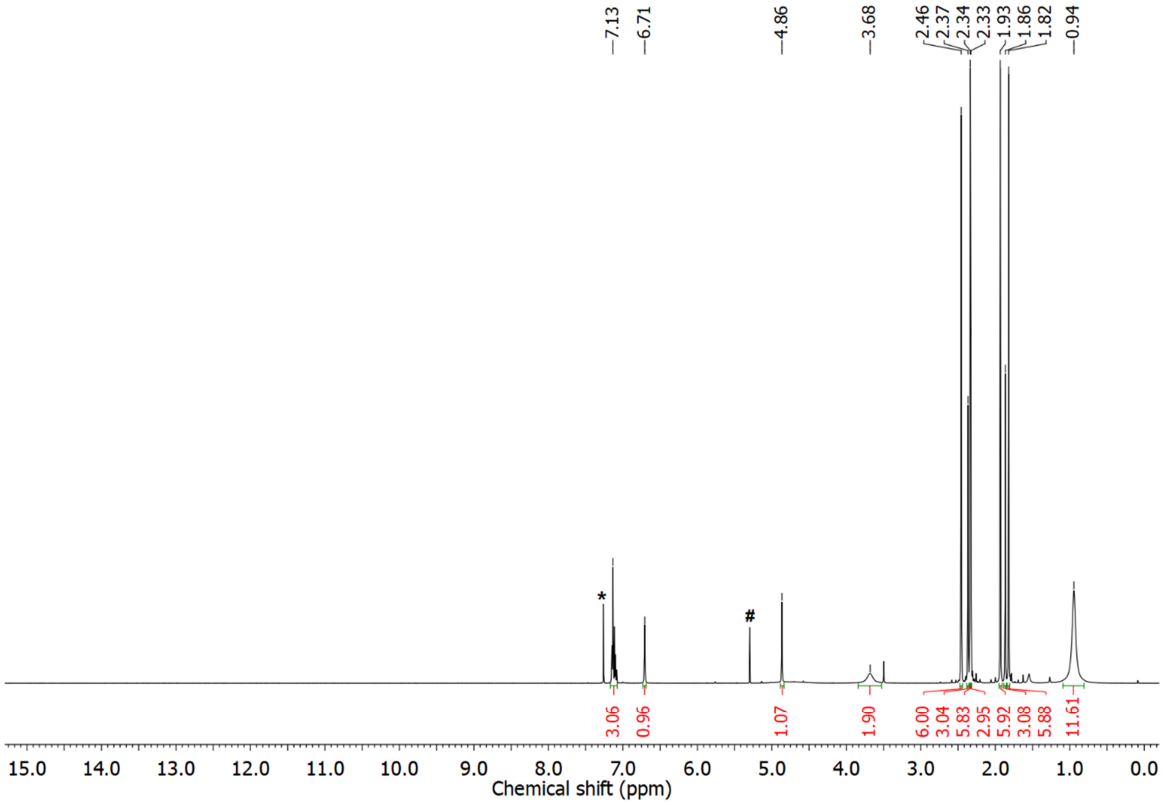


Figure S33. ^{1}H NMR spectrum of **9** in $CDCl_3$ (*), # CH_2Cl_2.

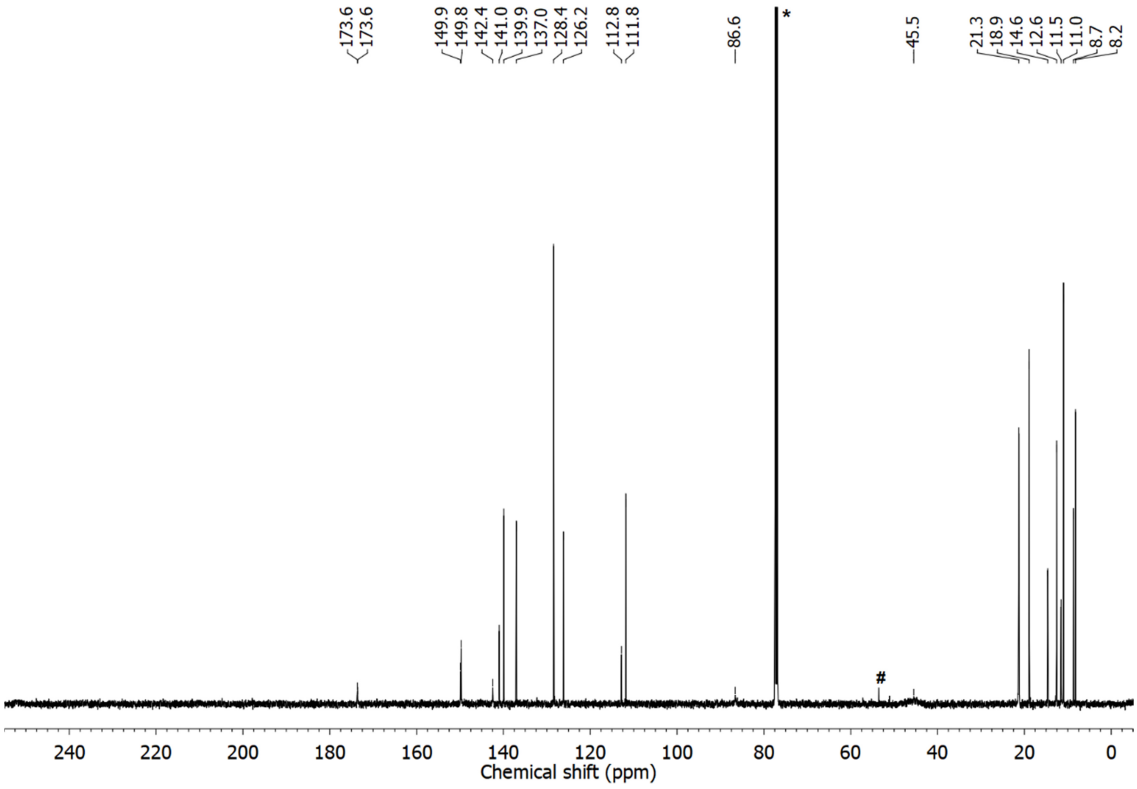


Figure S34. ^{13}C NMR spectrum of **9** in $CDCl_3$ (*), # CH_2Cl_2.

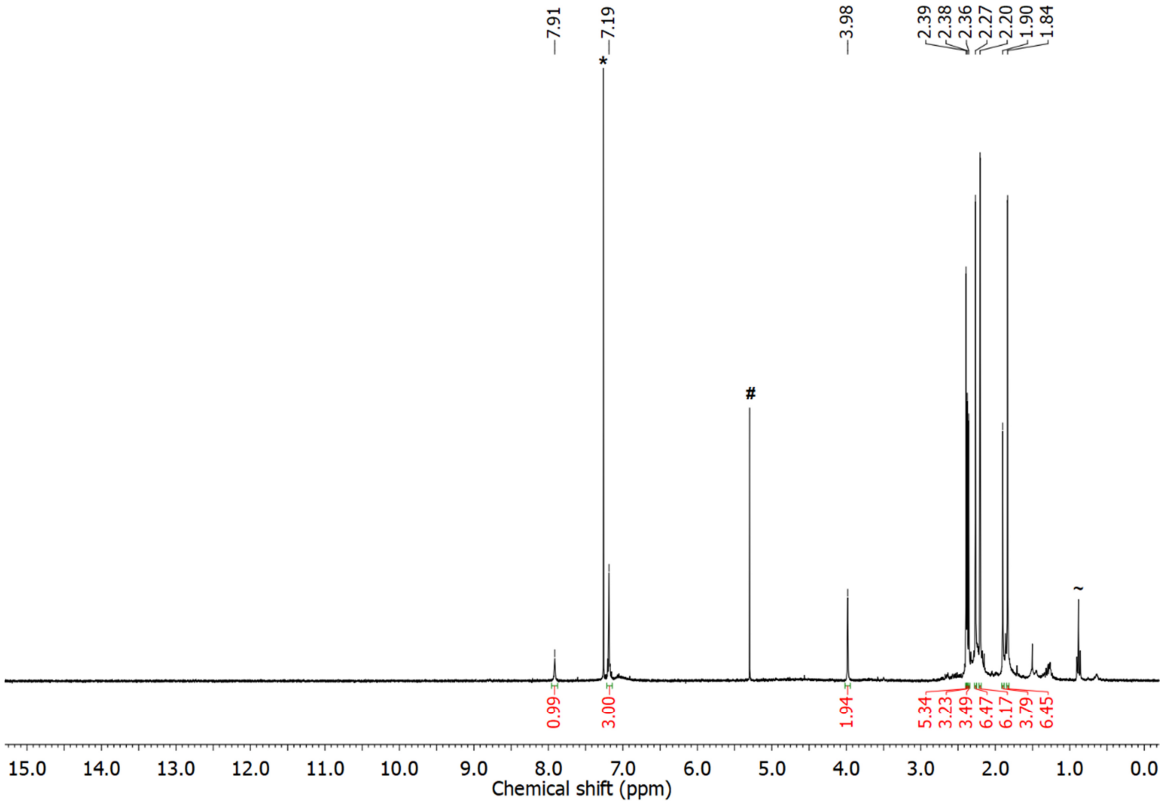


Figure S35. ^{1}H NMR spectrum of **10** in $CDCl_3$ (*), # CH_2Cl_2, ~ *n*-pentane.

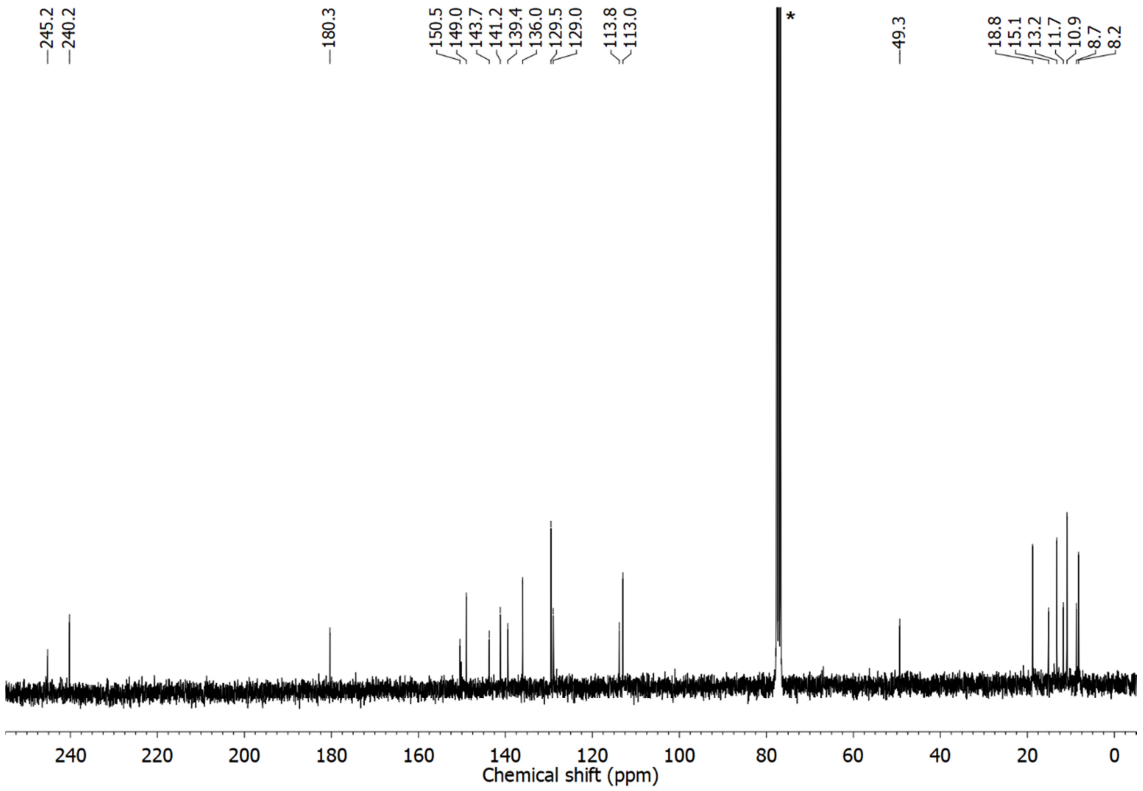


Figure S36. ^{13}C NMR spectrum of **10** in $CDCl_3$ (*).

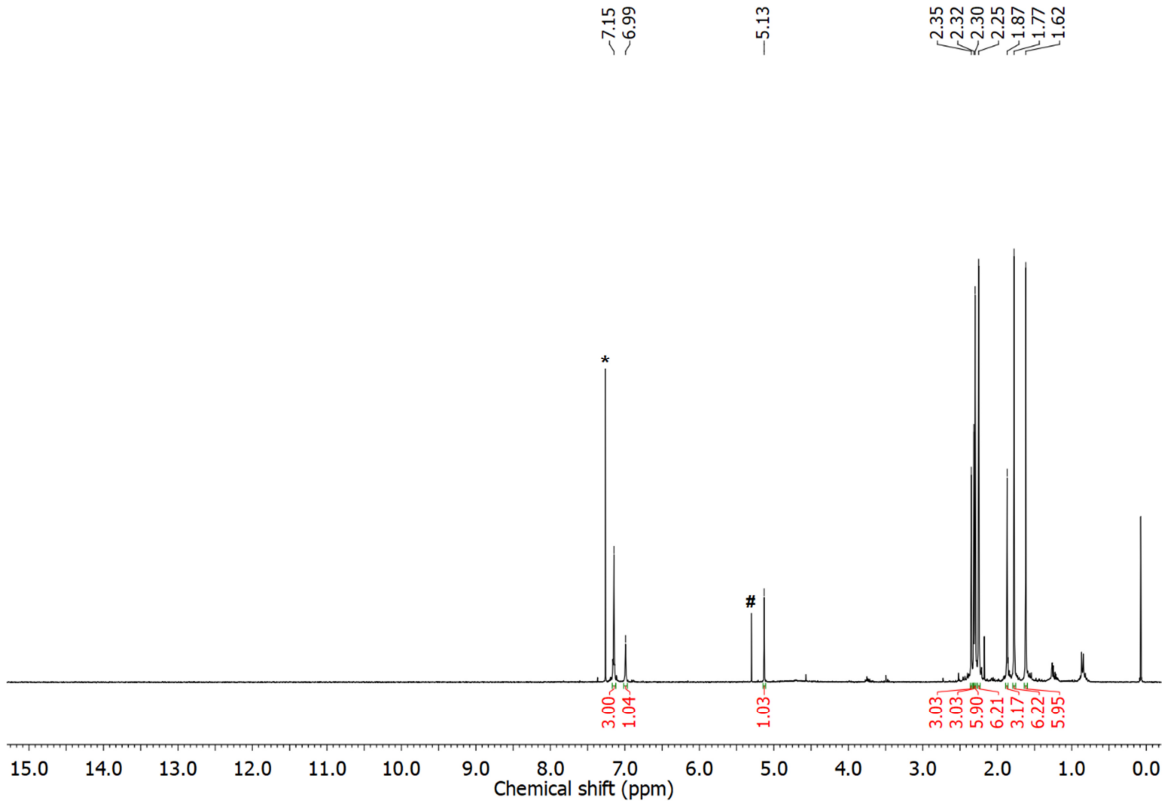


Figure S37. ^{1}H NMR spectrum of **11** in $CDCl_3$ (*), # CH_2Cl_2.

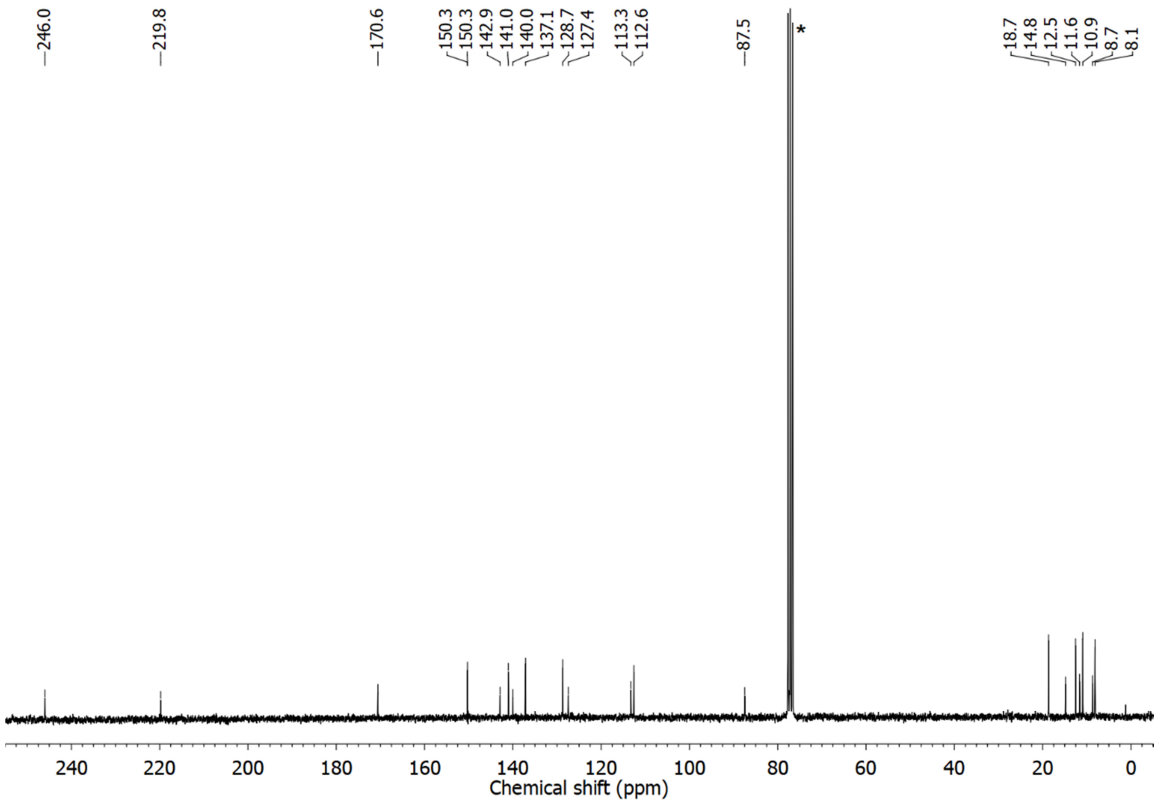


Figure S38. ^{13}C NMR spectrum of **11** in $CDCl_3$ (*).

11. Spectroscopic details for the UV irradiation of 4a

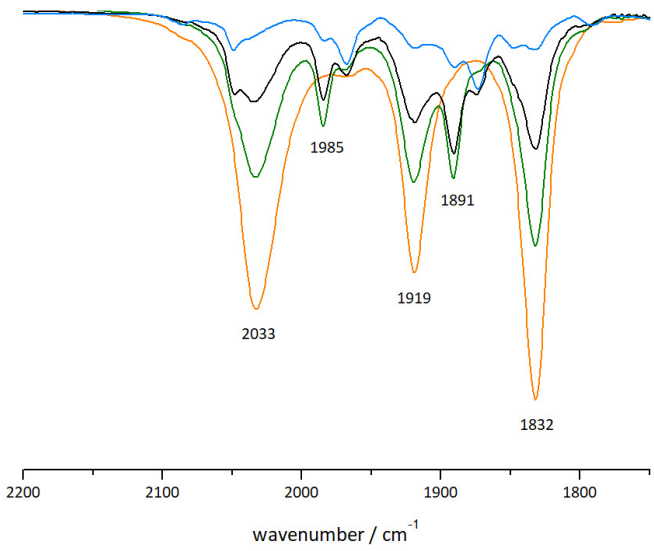


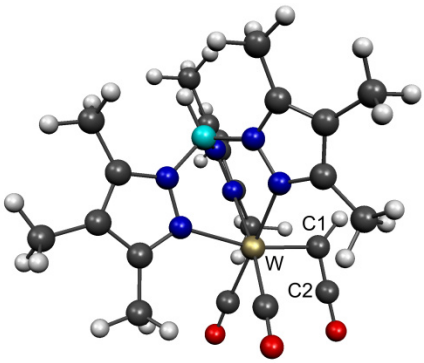
Figure S39. Selected IR spectra of compound **4a** (orange) after 1 h (green), 2 h (black) and 3 h (blue) of irradiation with UV light in toluene solution. Bands at 1985 and 1891 cm^{-1} are assigned to the methylidyne complex [Tp*W(CO)$_2$CH].

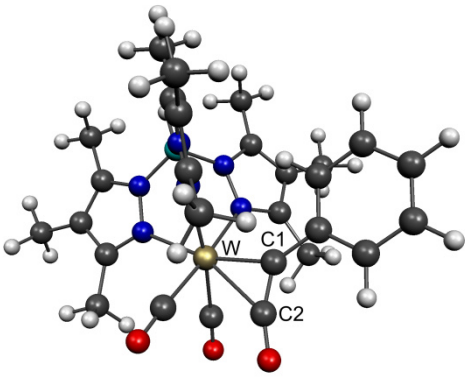
12. Computation details

DFT calculations were carried out as closed shell (S = 0) calculations using the G09RevE.01[S3] program package. Molecular geometries were optimized without truncation and symmetry constraints in the gas phase using either the PBE0[S4] or the M06[S5] functional. Quasi-relativistic effective core potentials of the Stuttgart/Cologne group were used for W (ECP60MBW) in combination with a (8s7p6d2f1g)/[6s5p3d2f1g] basis set.[S6] Split valence triple ζ-basis sets (def2-TZVP) of the Ahlrich group were used for the other elements.[S7] Dispersion was accounted for by the atom-pairwise dispersion correction with the Becke-Johnson damping scheme (D3BJ).[S8] In doing so a reasonable match between the calculated and the experimentally determined structures for **4b** and **8** were achieved (Table S3). Frequency calculations were performed to identify all stationary points as minima. The molecular structures are depicted in Figures S40 to S42 and the cartesian coordinates are given in Table S5 to S9. Transition states have been calculated using the nudged elastic band method (NEB) and subsequent optimization to a saddle point (OptTS) as implemented in orca 4.11.[S9] Corresponding geometry optimizations were performed with the low cost combination of BP86[S10] functional and def2-SVP basis set. Frequency calculations resulted one imaginary mode, respectively, at –200.81 cm^{-1} for the transition state **IM1** to **IM2** and –195.35 cm^{-1} for the transition state **IM2** to **IM3**. A Gibbs energy diagram is given in Figure S43. It should be noted, that the energy values are more reliable for the M06 functional and the def2-TZVP basis set.

Table S3. Comparison of calculated and experimentally determined structure data for **4b** and **8**.

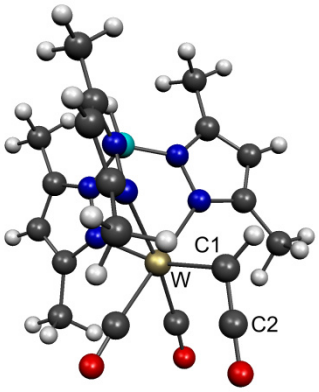
	4b				**8**	
	calc. (BPE0)	calc. (M06)	exp. (XRD)		calc. (M06)	exp. (XRD)
W–C1	2.050	2.074	2.053(3)	W–C1	2.184	2.189(3)
				W–O1	2.112	2.110(2)
W–N (*trans*-CO)	2.231	2.254	2.2061(18)	W–N (*trans*-CO)	2.268	2.248(2)
W–N (*trans*-CO)	2.234	2.265	2.2224(18)	W–N (*trans*-CO)	2.269	2.244(2)
W–N (*trans*-Ketenyl)	2.195	2.215	2.176(2)	W–N (*trans*-cycle)	2.250	2.225(2)
W–CO	1.963	1.988	1.981(2)	W–CO	1.976	1.958(3)
	1.961	1.981	1.954(2)		1.976	1.962(3)
				C1–C2 (chelate ring)	1.402	1.401(4)
C1–C2	1.319	1.314	1.307(4)	C2–C3 (chelate ring)	1.383	1.369(4)
				C3–O1	1.263	1.281(3)

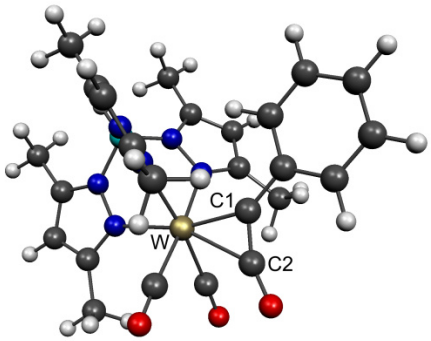




W–C1 2.056		W–C1 2.026
W–C2 2.666		W–C2 2.316
C1–C2 1.318		C1–C2 1.338
2167, 2028, 1948 cm^{-1}	IR	2085, 1987, **1970** cm^{-1}

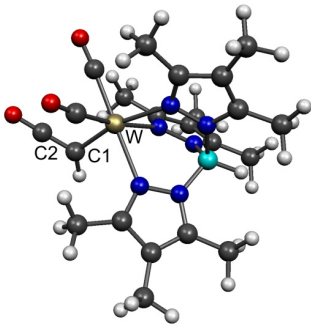
Figure S40. Calculated structures of **4a** (left) and **4a**-Ph (right); selected bond lengths and uncorrected CO-stretching frequencies, bold: mainly ketenyl stretch.



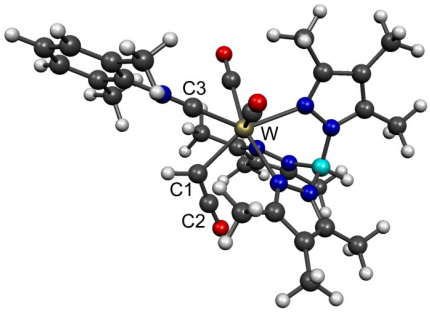


W–C1 2.059		W–C1 2.032
W–C2 2.687		W–C2 2.300
C1–C2 1.319		C1–C2 1.343
2168, 2030, 1951 cm^{-1}	IR	2086, 1990, **1968** cm^{-1}

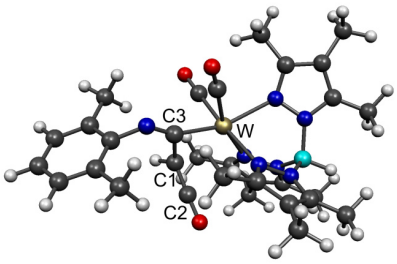
Figure S41. Calculated structures of **4b** (left) and **4b**-Ph (right); selected bond lengths and uncorrected CO-stretching frequencies, bold: mainly ketenyl stretch.



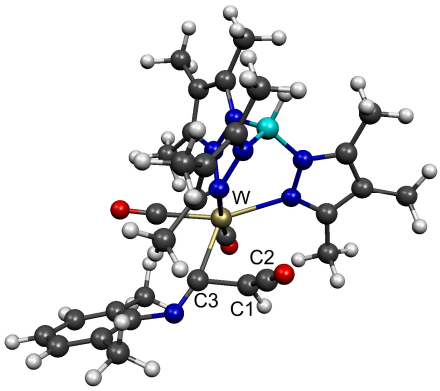
W–C1 2.074
W–C2 2.726
C1–C2 1.314



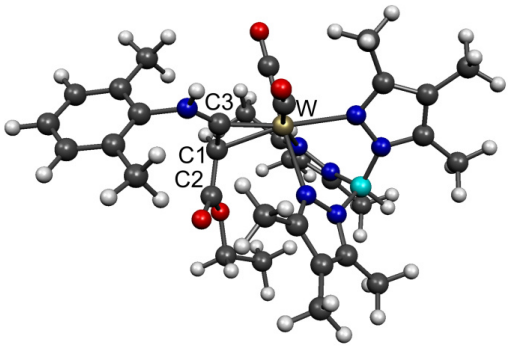
W–C1 2.258
W–C3 2.015
C1–C3 2.489



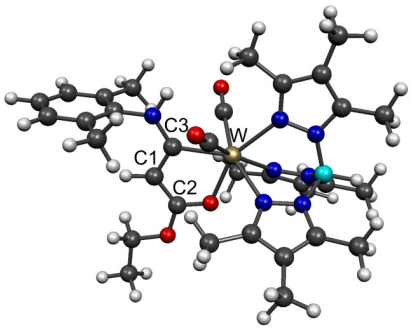
W–C1 2.301
W–C3 2.055
C1–C3 1.561



W–C1 2.282
W–C3 2.074
C1–C3 1.561



W–C3 2.232
C1–C2 2.016
C1–C3 1.425



W–C3 2.184
C1–C2 1.383
C1–C3 1.402

Figure S42. Optimized structures of **4a**, **IM1** and **IM2'** (upper row left to right), **IM2** and **IM3** (middle row left to right) and **8** (bottom) {DFT, M06, def2-TZVP, ECP60(W)}, selected calculated bond length.

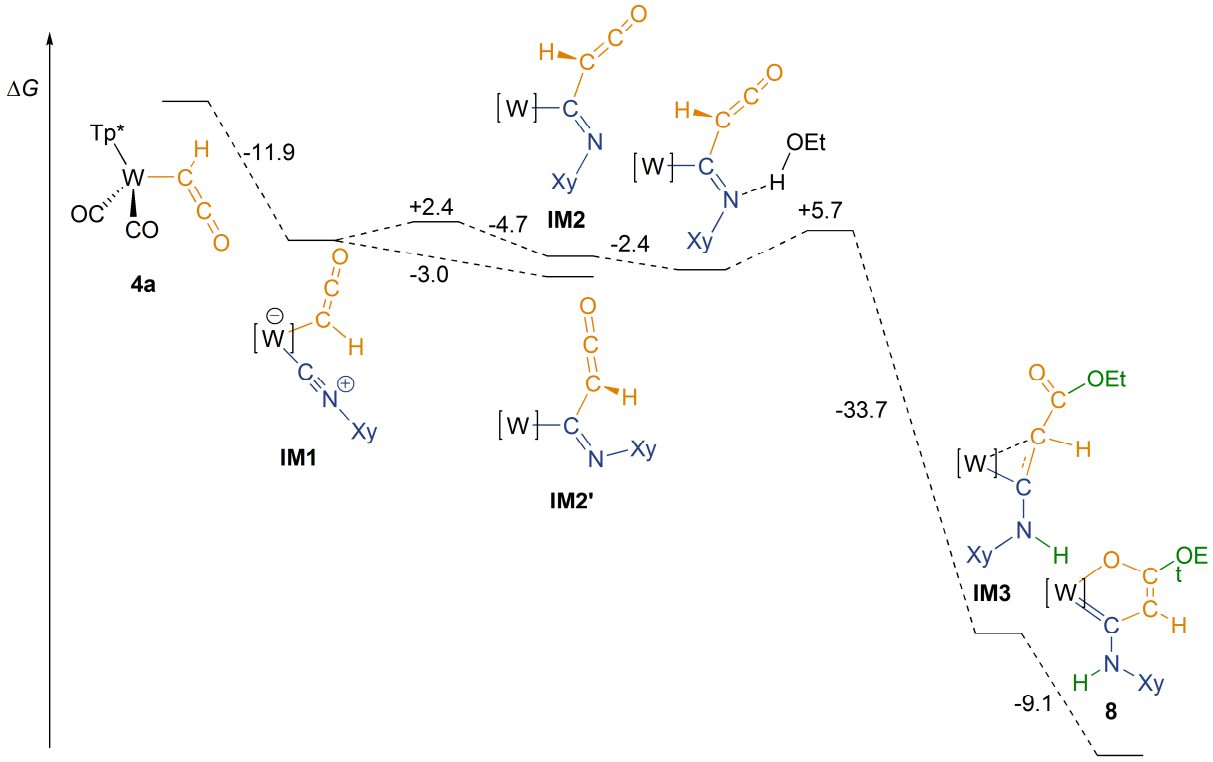


Figure S43. Reaction profile with calculated Gibbs energies ΔG_{298} in kcal/mol (BP86/def2-SVP).

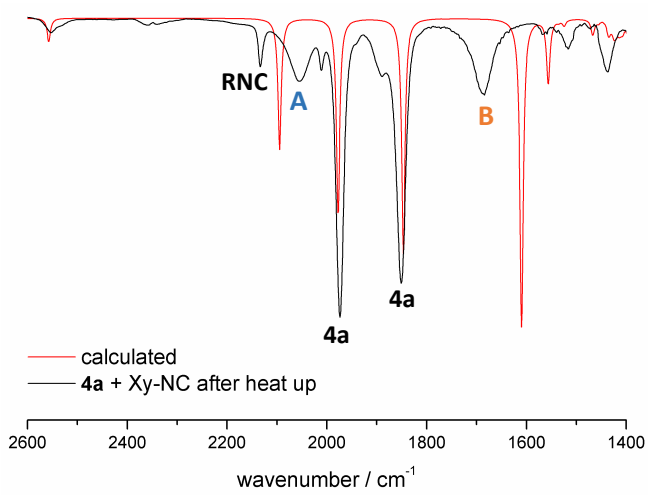


Figure S44. Selected IR spectrum of **4a** in THF solution with Xy-NC after heat up to rt. (black) and the calculated IR spectrum (red) of the intermediate **IM2'** (see Fig. S42).

Table S4. Selected wavenumbers of the intermediate **IM2'** from Fig. S42 experimental versus calculated.

	exp. (black)	calc. (red)
C=C=O (**A**)	2055	2095
C=N (**B**)	1687	1611
C≡O (**4**)	1974, 1851	1978, 1844

13. Cartesian coordinates of calculated complexes

Table S5. Cartesian coordinates of the geometry optimized structures of **4b** (left) and **4a** (right) in the gas phase; BPE0, def2-TZVP/ECP(W) with empirical dispersion correction (GD3BJ).

W	-1.023238	0.000093	-0.029311	W	1.16381	0.00085	-0.03097
N	0.448289	1.493155	-0.817319	N	-0.30483	-1.49881	-0.80908
N	0.402722	0.001916	1.649385	N	-0.25992	0.01065	1.64688
N	0.447698	-1.495341	-0.813551	N	-0.30897	1.48722	-0.82877
C	-1.922298	-0.001663	-1.881449	C	2.06071	-0.00708	-1.88539
C	-2.317854	-1.199875	0.853203	C	2.45806	1.20678	0.84387
C	-2.317183	1.202495	0.850898	C	2.46156	-1.19231	0.85533
H	-1.516751	-0.002810	-2.886971	H	1.65282	-0.01115	-2.88984
N	1.777794	1.255170	-0.752760	N	-1.63105	-1.26388	-0.74398
C	0.284661	2.682838	-1.405479	C	-0.14066	-2.68723	-1.3979
N	1.742314	0.001904	1.409657	N	-1.59587	0.00868	1.40884
C	0.242308	0.003785	2.985979	C	-0.09976	0.02066	2.98296
N	1.777314	-1.257887	-0.748949	N	-1.6344	1.24841	-0.76292
C	0.283742	-2.686421	-1.398781	C	-0.14794	2.66811	-1.43327
C	-3.209205	-0.001500	-1.592624	C	3.34747	-0.00572	-1.59849
O	-3.124697	-1.823109	1.398914	O	3.26556	1.83279	1.3862
O	-3.123784	1.826815	1.395725	O	3.27109	-1.81095	1.4032
B	2.287570	-0.000376	-0.034519	B	-2.14205	-0.00298	-0.03531
C	2.461797	2.276086	-1.296258	C	-2.31304	-2.28819	-1.28869
C	1.536615	3.206656	-1.730045	C	-1.39121	-3.22668	-1.72849
C	-1.043896	3.298499	-1.647476	C	1.19	-3.29706	-1.64206
C	2.418460	0.003723	2.564108	C	-2.27054	0.01733	2.56608
C	1.491019	0.004983	3.593777	C	-1.34706	0.02514	3.60715
C	-1.075208	0.004143	3.669131	C	1.22131	0.02605	3.65932

C	2.461031	-2.280543	-1.289514	C	-2.31909	2.26258	-1.32317
C	1.535570	-3.211730	-1.721380	C	-1.39982	3.19828	-1.77398
C	-1.045004	-3.301953	-1.640115	C	1.18095	3.27991	-1.68195
O	-4.345467	-0.001372	-1.355028	O	4.48459	-0.00465	-1.36302
H	3.483714	-0.000604	-0.011768	H	-3.33763	-0.00441	-0.01204
C	3.944743	2.325935	-1.373799	C	-3.79706	-2.32132	-1.35677
H	1.741354	4.148732	-2.212809	H	1.70467	-2.81463	-2.4771
H	-1.590639	2.772362	-2.433169	H	1.07879	-4.35597	-1.87887
H	-0.919434	4.338207	-1.951440	H	1.83815	-3.20105	-0.77008
H	-1.665596	3.267603	-0.751315	C	-3.75472	0.01787	2.63626
C	3.901181	0.004361	2.656097	H	1.81599	-0.85047	3.39824
H	1.697638	0.006496	4.651810	H	1.07766	0.02596	4.74006
H	-1.667172	0.882703	3.409158	H	1.80864	0.90759	3.39798
H	-0.919564	0.005825	4.748249	C	-3.80308	2.28922	-1.39465
H	-1.666164	-0.875872	3.411759	H	1.83005	3.18931	-0.81015
C	3.944002	-2.331602	-1.365881	H	1.06699	4.33746	-1.92366
H	1.740041	-4.155192	-2.201542	H	1.69593	2.79511	-2.51544
H	-1.667007	-3.269490	-0.744222	H	-4.24883	-2.31806	-0.36199
H	-0.920842	-4.342177	-1.942427	H	-4.12649	-3.2237	-1.87092
H	-1.591280	-2.776776	-2.426789	H	-4.19588	-1.46138	-1.89943
H	4.403265	2.316830	-0.382342	H	-4.17991	0.89589	2.14548
H	4.251195	3.240994	-1.880194	H	-4.07921	0.02306	3.67603
H	4.349801	1.477401	-1.929581	H	-4.18036	-0.86444	2.15373
H	4.334984	-0.875765	2.176920	H	-4.19758	1.42026	-1.92599
H	4.199823	0.004533	3.704059	H	-4.1348	3.18304	-1.9221
H	4.334137	0.884953	2.176955	H	-4.25687	2.29813	-0.40081

H	4.350309	-1.483297	-1.921056	C	-1.64681	-4.53091	-2.40105
H	4.250080	-3.246844	-1.872176	H	-1.24019	-4.55245	-3.41626
H	4.401664	-2.323215	-0.373997	H	-1.19389	-5.36235	-1.85356
				H	-2.71509	-4.7388	-2.47532
				C	-1.65864	4.49192	-2.46547
				H	-1.20554	5.33196	-1.93144
				H	-1.2542	4.49881	-3.48177
				H	-2.72735	4.69738	-2.54046
				C	-1.61102	0.03674	5.07337
				H	-1.16619	-0.8293	5.57097
				H	-1.20289	0.93162	5.55131
				H	-2.68054	0.01658	5.28604

Table S6. Cartesian coordinates of the geometry optimized structures of **4b**-Ph (left) and **4a**-Ph (right) in the gas phase; BPE0, def2-TZVP/ECP(W) with empirical dispersion correction (GD3BJ).

W	0.068138	-1.007309	-0.000121	W	-0.139568	-1.139850	-0.000128
N	-0.164707	0.639107	-1.495279	N	0.078505	0.500112	-1.485923
N	-2.162387	-0.814560	-0.000100	N	-2.219504	-0.377468	0.000203
N	-0.164745	0.638650	1.495419	N	0.078947	0.500279	1.485530
C	2.073998	-0.682211	-0.000101	C	1.880887	-1.286152	-0.000103
C	0.002148	-2.525315	1.277414	C	-0.570530	-2.602758	1.268701
C	0.002372	-2.525027	-1.278068	C	-0.570405	-2.602753	-1.268968
N	-0.988630	1.685552	-1.256769	N	-0.432255	1.725353	-1.249031
C	0.410323	0.845919	-2.684671	C	0.757213	0.564306	-2.634814
N	-2.735265	0.417026	0.000009	N	-2.450875	0.956821	0.000264
C	-3.160875	-1.713329	-0.000211	C	-3.416058	-0.986440	0.000591
N	-0.988684	1.685153	1.257219	N	-0.431718	1.725548	1.248543

C	0.410272	0.845099	2.684882	C	0.757953	0.564612	2.634221
C	2.130786	-2.024485	0.000459	C	1.654833	-2.604760	-0.000049
O	-0.022844	-3.453593	1.958168	O	-0.817561	-3.504745	1.941088
O	-0.022113	-3.452505	-1.959924	O	-0.817327	-3.504756	-1.941382
B	-1.868454	1.691183	0.000208	B	-1.286651	1.960651	-0.000076
C	-0.943738	2.555461	-2.280513	C	-0.082961	2.573066	-2.233768
C	-0.054155	2.052015	-3.210256	C	0.687657	1.867703	-3.146255
C	1.384582	-0.091325	-3.296691	C	1.471032	-0.593043	-3.223889
C	-4.070731	0.307687	-0.000065	C	-3.769676	1.197454	0.000704
C	-4.378523	-1.041324	-0.000211	C	-4.430371	-0.025965	0.000920
C	-2.964848	-3.185213	-0.000263	C	-3.594425	-2.459081	0.000728
C	-0.943819	2.554739	2.281240	C	-0.082064	2.573405	2.233041
C	-0.054229	2.051023	3.210834	C	0.688709	1.868120	3.145436
C	1.384611	-0.092295	3.296544	C	1.471889	-0.592619	3.223384
O	2.618111	-3.107755	0.000748	O	1.873696	-3.771132	-0.000011
H	-2.571817	2.658238	0.000346	H	-1.711845	3.077230	-0.000060
C	-1.743031	3.806923	-2.333639	C	-0.506324	3.995757	-2.250766
H	0.221212	2.497922	-4.152400	H	2.427538	-0.762040	-2.722291
H	2.317336	-0.119988	-2.729573	H	1.671981	-0.409864	-4.279992
H	1.611703	0.227158	-4.314288	H	0.888865	-1.509825	-3.132979
H	0.992753	-1.109077	-3.331393	C	-4.334281	2.570111	0.000859
C	-4.995029	1.470855	0.000047	H	-3.144754	-2.923106	-0.878018
H	-5.362323	-1.482025	-0.000288	H	-4.657915	-2.697700	-0.000274
H	-2.415588	-3.523376	-0.879803	H	-3.146553	-2.922660	0.880651
H	-3.938239	-3.676180	-0.000923	C	-0.505357	3.996119	2.249935
H	-2.416714	-3.523566	0.879919	H	0.890807	-1.509873	3.130538

C	-1.743121	3.806177	2.334752	H	1.670841	-0.410289	4.280022
H	0.221160	2.496668	4.153096	H	2.429452	-0.760127	2.723277
H	0.992806	-1.110066	3.331015	H	-1.594145	4.091839	-2.271928
H	1.611854	0.225921	4.314197	H	-0.106659	4.493238	-3.133625
H	2.317292	-0.120796	2.729296	H	-0.148093	4.533357	-1.369931
H	-2.816059	3.602307	-2.330995	H	-4.017354	3.133076	0.881219
H	-1.504533	4.351325	-3.247104	H	-5.422534	2.526414	0.000811
H	-1.532292	4.459551	-1.483663	H	-4.017317	3.133261	-0.879371
H	-4.850446	2.100263	0.880640	H	-0.149293	4.533005	1.367806
H	-6.025289	1.115921	0.000020	H	-0.103585	4.494278	3.131455
H	-4.850460	2.100436	-0.880425	H	-1.593138	4.092230	2.273690
H	-1.532510	4.458996	1.484893	C	3.084100	-0.487966	0.000066
H	-1.504506	4.350375	3.248309	C	3.025157	0.910328	-0.000207
H	-2.816147	3.601546	2.332211	C	4.340994	-1.106968	0.000518
C	3.116131	0.321760	-0.000036	C	4.186760	1.662128	-0.000006
C	2.811803	1.688007	-0.000245	H	2.059066	1.397477	-0.000570
C	4.464413	-0.063296	0.000234	C	5.499390	-0.351080	0.000725
C	3.821166	2.635139	-0.000211	H	4.391117	-2.190273	0.000713
H	1.773331	1.995241	-0.000448	C	5.426269	1.036170	0.000469
C	5.470038	0.886770	0.000277	H	4.126216	2.744640	-0.000215
H	4.708697	-1.120135	0.000429	H	6.464938	-0.843918	0.001086
C	5.152064	2.239093	0.000044	H	6.334550	1.627888	0.000632
H	3.569974	3.689964	-0.000384	C	-5.897334	-0.280221	0.001408
H	6.507882	0.572903	0.000483	H	-6.209145	-0.847658	-0.879568
H	5.941058	2.982702	0.000068	H	-6.208407	-0.848422	0.882147
				H	-6.461900	0.652761	0.002054

				C	1.321077	2.360775	4.399196
				H	0.987457	1.789817	5.270169
				H	2.411002	2.282556	4.357860
				H	1.075655	3.407209	4.584572
				C	1.319665	2.360327	-4.400212
				H	2.409801	2.285543	-4.357836
				H	0.988552	1.786959	-5.270539
				H	1.071165	3.405697	-4.587480

Table S7. Cartesian coordinates of the geometry optimized structures of **4a** (left) and **IM1** (right) in the gas phase; M06, def2-TZVP/ECP(W).

W	-1.175185	0.002266	0.030032	B	3.102057	-0.078621	-0.048221
B	2.154562	-0.049252	0.003735	H	4.292036	-0.148327	-0.048571
H	3.346972	-0.063128	-0.030140	N	1.155289	-1.598694	-0.503868
N	0.288624	-1.679369	0.362639	N	2.497593	-1.446881	-0.403499
N	1.623652	-1.453585	0.333535	N	1.326540	1.234425	-1.293177
N	0.346879	1.183713	1.220043	N	2.639906	0.959265	-1.099533
N	1.671977	0.950908	1.066481	N	1.288492	0.576440	1.558806
N	0.256227	0.475625	-1.592797	N	2.608620	0.372614	1.335895
N	1.598572	0.385413	-1.374004	O	-1.404347	-0.564111	-2.905411
O	-3.350845	-1.315718	-1.800742	O	-1.231130	3.065287	0.525677
C	-2.080909	-0.459845	1.837139	W	-0.247578	0.135825	-0.063456
H	-1.639144	-0.702639	2.796929	C	-0.997804	-0.285238	-1.865151
C	-3.370917	-0.397733	1.594844	C	-0.884402	1.993524	0.288888
O	-4.501598	-0.333774	1.351138	C	0.927555	-2.858320	-0.875717
C	-2.467743	1.414192	-0.507159	C	2.141449	-3.539341	-1.014859
O	-3.279774	2.147382	-0.877225	C	3.112299	-2.607937	-0.704598

C	-2.512863	-0.892260	-1.126092	C	-0.421995	-3.426390	-1.095605
C	0.116262	-2.979748	0.606729	H	-0.607799	-3.594565	-2.160853
C	1.358707	-3.607596	0.746808	H	-1.196464	-2.768255	-0.704189
C	2.289298	-2.601561	0.559726	H	-0.512021	-4.392629	-0.592631
C	-1.217709	-3.613276	0.710447	C	2.297552	-4.963324	-1.403740
H	-1.680934	-3.417768	1.681337	H	3.347399	-5.252284	-1.466761
H	-1.132145	-4.694231	0.592005	H	1.844141	-5.168558	-2.377967
H	-1.901384	-3.232543	-0.049746	H	1.818425	-5.631980	-0.682590
C	1.593308	-5.047538	1.028112	C	4.585269	-2.762223	-0.669718
H	2.658328	-5.275552	1.087251	H	4.986825	-2.556013	0.324910
H	1.168596	-5.687645	0.249686	H	5.082780	-2.084717	-1.367360
H	1.142597	-5.355608	1.975405	H	4.862081	-3.781627	-0.937143
C	3.769229	-2.671748	0.578114	C	1.254910	2.181219	-2.230022
H	4.199830	-2.373016	-0.380509	C	2.542676	2.527109	-2.654653
H	4.096578	-3.689165	0.790137	C	3.390535	1.729137	-1.912711
H	4.195511	-2.015819	1.340651	C	-0.011609	2.784398	-2.707997
C	0.221771	2.136075	2.145173	H	-0.815198	2.052857	-2.782600
C	1.485670	2.522168	2.607483	H	0.136031	3.230304	-3.692590
C	2.378667	1.746975	1.891439	H	-0.353708	3.576686	-2.036384
C	-1.084659	2.676618	2.586483	C	2.884111	3.543189	-3.683116
H	-1.785257	2.762971	1.754893	H	2.529270	4.539213	-3.404048
H	-0.951371	3.662988	3.033752	H	2.437405	3.304962	-4.652660
H	-1.556060	2.033606	3.334803	H	3.962020	3.614664	-3.833368
C	1.769514	3.551641	3.640264	C	4.870389	1.658356	-1.936446
H	1.285986	3.315914	4.592166	H	5.305372	1.932456	-0.972595
H	1.412540	4.540303	3.337619	H	5.266102	2.341490	-2.687631

H	2.839242	3.641214	3.834068	H	5.224166	0.653431	-2.176729
C	3.859411	1.725007	1.942654	C	1.162000	1.010329	2.811842
H	4.241108	0.728857	2.177360	C	2.421313	1.086736	3.417091
H	4.221373	2.411417	2.707649	C	3.311350	0.672254	2.446521
H	4.301990	2.023204	0.989110	C	-0.129230	1.356460	3.448208
C	0.097758	0.893183	-2.859819	H	-0.227738	0.840822	4.407209
C	1.341010	1.073083	-3.461211	H	-0.975082	1.071412	2.824566
C	2.265180	0.737872	-2.481586	H	-0.186587	2.430288	3.650633
C	-1.220942	1.135294	-3.488426	C	2.686275	1.521410	4.811538
H	-1.917886	0.315382	-3.316057	H	3.751588	1.504428	5.045124
H	-1.100915	1.259768	-4.564999	H	2.183730	0.875049	5.537061
H	-1.689388	2.042531	-3.099874	H	2.329415	2.539606	4.992765
C	1.595567	1.528485	-4.852816	C	4.784816	0.537111	2.517031
H	2.663380	1.581424	-5.067952	H	5.139977	0.814431	3.509256
H	1.178766	2.522107	-5.037303	H	5.287985	1.177540	1.789000
H	1.150827	0.853389	-5.588950	H	5.103637	-0.489189	2.321696
C	3.744864	0.738885	-2.556110	C	-0.929026	-1.312216	1.529484
H	4.182665	1.427860	-1.830414	H	-1.937306	-1.458785	1.895707
H	4.074230	1.042547	-3.549019	C	0.014712	-1.992118	2.103535
H	4.158201	-0.250879	-2.350739	O	0.918669	-2.564770	2.570385
				C	-2.260129	0.158047	0.025151
				C	-4.798301	0.043216	0.055655
				C	-5.625264	1.146557	0.291054
				C	-5.312287	-1.233598	-0.201617
				C	-6.995798	0.943859	0.268266
				C	-6.689154	-1.385451	-0.210174

				C	-7.527546	-0.309477	0.022875
				H	-7.652385	1.788296	0.449206
				H	-7.105833	-2.367862	-0.405990
				H	-8.602129	-0.448552	0.011764
				N	-3.437518	0.217341	0.085653
				C	-4.391724	-2.375507	-0.466167
				H	-3.777979	-2.190108	-1.353151
				H	-3.696852	-2.535667	0.363763
				H	-4.949849	-3.297749	-0.626792
				C	-5.030555	2.490286	0.541819
				H	-4.298735	2.462175	1.353400
				H	-4.495187	2.855653	-0.339064
				H	-5.801375	3.218026	0.795295

Table S8. Cartesian coordinates of the geometry optimized structures of **IM2** (left) and **IM2'** (right) in the gas phase; M06, def2-TZVP/ECP(W).

B	2.804976	0.545609	-0.760344	B	2.884385	0.659290	0.548126
H	3.890184	0.865847	-1.188903	H	3.968898	1.040296	0.863548
N	-3.207750	0.494796	1.211222	N	-3.204104	0.105440	-1.038669
N	1.867284	-0.231604	1.450966	N	1.099359	-0.810100	1.544373
N	2.924361	0.242589	0.748383	N	2.295859	-0.189150	1.690473
N	1.166789	-1.357871	-1.139815	N	1.915912	-0.851988	-1.249280
N	2.315772	-0.728031	-1.492617	N	2.995614	-0.214185	-0.723384
N	0.506411	1.524378	-0.627690	N	0.723955	1.664595	-0.223525
N	1.800011	1.682061	-0.991305	N	1.979441	1.859120	0.253718
O	-0.768210	-3.151899	1.809980	O	-0.963492	-3.474079	-0.564973
O	-2.276195	-0.856443	-1.888866	O	-1.007152	-0.181416	-3.364681

O	0.226125	2.775287	2.270656	O	-1.238822	1.876800	2.299961
W	-0.145378	-0.426576	0.415132	W	-0.098919	-0.487210	-0.349921
C	-0.544270	-2.136815	1.278501	C	-0.639826	-2.363467	-0.473359
C	-1.513956	-0.736048	-1.033664	C	-0.643985	-0.294450	-2.287004
C	-1.977480	0.265700	1.096787	C	-2.099037	-0.028002	-0.466972
C	-0.998929	0.606620	2.262564	C	-1.881569	-0.173848	1.071614
H	-1.205064	0.132798	3.232470	H	-2.432384	-0.947842	1.601153
C	-0.360707	1.780782	2.278210	C	-1.553659	0.924279	1.741322
C	-4.313479	0.135746	0.444887	C	-4.455652	0.058834	-0.414456
C	-4.662025	-1.218333	0.228141	C	-5.156933	1.239106	-0.153063
C	-5.818577	-1.502034	-0.499995	C	-6.418565	1.153423	0.418387
H	-6.082814	-2.552145	-0.668065	H	-6.961931	2.071202	0.621623
C	-6.638530	-0.491915	-0.991517	C	-6.985357	-0.069700	0.723256
H	-7.538871	-0.739178	-1.561270	H	-7.974446	-0.119641	1.163173
C	-6.319608	0.833259	-0.718119	C	-6.283974	-1.229720	0.450553
H	-6.978068	1.639397	-1.060927	H	-6.724003	-2.196685	0.674659
C	-5.178771	1.167576	0.012676	C	-5.019927	-1.190020	-0.120276
C	-3.850199	-2.334835	0.802066	C	-4.549447	2.563229	-0.473934
H	-2.949183	-2.558472	0.205163	H	-3.737433	2.808505	0.218700
H	-4.441255	-3.261628	0.850656	H	-5.291130	3.360309	-0.406793
H	-3.496064	-2.100791	1.819301	H	-4.115917	2.567647	-1.477022
C	-4.889744	2.597609	0.345767	C	-4.277991	-2.448304	-0.431243
H	-4.253382	3.084247	-0.413462	H	-3.412267	-2.596647	0.221975
H	-4.358526	2.677623	1.307805	H	-3.882931	-2.437159	-1.450224
H	-5.820357	3.183546	0.402032	H	-4.924383	-3.319138	-0.317027
C	2.302180	-0.484940	2.695002	C	0.901644	-1.533485	2.650564

C	3.665829	-0.155200	2.801540	C	1.974695	-1.366246	3.530459
C	4.021868	0.298012	1.535066	C	2.841853	-0.511126	2.877049
C	1.461546	-1.027024	3.793315	C	-0.281284	-2.390825	2.897776
H	2.079730	-1.633446	4.473315	H	0.025663	-3.323858	3.375486
H	0.643720	-1.660144	3.423809	H	-0.808193	-2.638494	1.978754
H	1.019248	-0.220279	4.404387	H	-0.988217	-1.906057	3.578778
C	4.511711	-0.286075	4.019358	C	2.116302	-1.997894	4.866995
H	5.544340	0.046697	3.835567	H	3.015513	-1.655314	5.380393
H	4.566844	-1.330584	4.372227	H	2.177770	-3.087994	4.797759
H	4.121907	0.313668	4.859580	H	1.265511	-1.767888	5.514462
C	5.341446	0.770051	1.043756	C	4.157524	0.006972	3.320009
H	5.280954	1.784527	0.618218	H	4.174168	1.098631	3.345920
H	5.746160	0.112893	0.256650	H	4.961932	-0.312744	2.653570
H	6.069314	0.792867	1.867246	H	4.386751	-0.357324	4.321008
C	1.070784	-2.467626	-1.888734	C	2.356095	-1.582418	-2.278133
C	2.176472	-2.550986	-2.755827	C	3.734697	-1.408053	-2.430969
C	2.944645	-1.427765	-2.463847	C	4.100027	-0.539075	-1.420746
C	-0.046140	-3.442738	-1.795062	C	1.491879	-2.440019	-3.121363
H	-0.371508	-3.595358	-0.755442	H	0.697190	-2.909943	-2.543563
H	0.268542	-4.415146	-2.202390	H	2.089869	-3.226082	-3.584630
H	-0.929641	-3.117543	-2.370909	H	1.020244	-1.870265	-3.926366
C	2.439907	-3.624960	-3.753078	C	4.589610	-2.044073	-3.465891
H	1.620046	-3.718607	-4.485199	H	4.250905	-1.800465	-4.476424
H	2.556992	-4.613531	-3.276290	H	4.585560	-3.134614	-3.382003
H	3.361429	-3.431697	-4.322899	H	5.627490	-1.719045	-3.384109
C	4.236648	-0.993989	-3.054174	C	5.441311	-0.008172	-1.081073

H	4.172972	0.022264	-3.476316	H	5.440387	1.082658	-1.030427
H	4.535237	-1.675901	-3.862622	H	6.167988	-0.311963	-1.833926
H	5.047960	-0.982642	-2.308137	H	5.789452	-0.375063	-0.112202
C	-0.157109	2.599341	-1.073286	C	0.258810	2.865988	-0.567393
C	0.726750	3.474186	-1.735232	C	1.216940	3.852562	-0.304235
C	1.964778	2.844179	-1.663903	C	2.298915	3.168260	0.209313
C	-1.613591	2.801009	-0.874711	C	-1.084713	3.107206	-1.135962
H	-1.864598	3.066294	0.167141	H	-1.751965	3.540712	-0.384557
H	-2.193660	1.898417	-1.122802	H	-1.548365	2.195671	-1.507953
H	-1.971563	3.623747	-1.511949	H	-1.027023	3.824492	-1.957967
C	0.380223	4.778280	-2.364985	C	1.056342	5.308948	-0.543734
H	1.251209	5.236324	-2.857773	H	1.944046	5.867615	-0.244459
H	0.005336	5.509088	-1.628030	H	0.209526	5.719587	0.013674
H	-0.403535	4.668753	-3.134031	H	0.876334	5.527864	-1.600406
C	3.279028	3.275892	-2.204525	C	3.617210	3.683318	0.648546
H	3.182871	4.242595	-2.718729	H	3.646621	4.768837	0.558060
H	3.684487	2.549019	-2.927917	H	4.432422	3.274026	0.046468
H	4.033608	3.393481	-1.409590	H	3.826335	3.427364	1.689762

Table S9. Cartesian coordinates of the geometry optimized structures of **IM3** (left) and **8** (right) in the gas phase; M06, def2-TZVP/ECP(W).

B	2.900253	0.663092	-0.155808	B	3.390102	-0.039172	-0.004986
H	3.974437	1.177383	-0.212522	H	4.582169	-0.002481	-0.008808
N	-3.117375	-0.780742	-0.778924	N	-2.940279	-1.253553	-0.000014
N	1.273719	0.034151	1.661226	H	-2.499675	-2.162045	0.018501
N	2.417650	0.669939	1.308607	N	1.515779	0.746742	1.461159
N	1.948158	-1.657315	-0.622262	N	2.849672	0.662702	1.254152

N	3.005725	-0.799198	-0.653569	N	1.602058	-1.841617	-0.005521
N	0.673995	0.929694	-1.261079	N	2.917172	-1.509280	-0.010531
N	1.914444	1.433134	-1.038136	N	1.505901	0.754766	-1.456641
O	-0.681037	-3.383463	1.730335	N	2.840996	0.675184	-1.253737
O	-1.088287	-2.494827	-2.454445	O	-2.021873	3.428041	0.023919
O	-2.635348	2.444357	-0.148787	O	-0.921565	-1.805486	2.510219
W	-0.008835	-0.867927	0.026673	O	-0.936966	-1.790084	-2.503190
C	-0.442072	-2.430729	1.110082	O	-0.537180	1.822406	0.022783
C	-0.664443	-1.910026	-1.569798	W	0.059456	-0.203673	0.005747
C	-2.017425	-0.531876	-0.238634	C	-0.604290	-1.226066	1.560408
C	-1.879319	0.469910	0.999847	C	-0.612523	-1.217233	-1.551967
H	-2.793653	0.259843	1.563327	C	-2.124636	-0.171483	0.004578
C	-1.842771	1.909790	0.572374	C	-2.705822	1.104852	0.009705
C	-4.395724	-0.508601	-0.288883	H	-3.775753	1.266599	0.012569
C	-5.238458	0.366552	-0.986181	C	-1.765164	2.118703	0.018218
C	-6.520909	0.579096	-0.504767	C	-4.366034	-1.210429	-0.006880
H	-7.169216	1.264948	-1.041312	C	-5.040620	-1.150555	-1.227176
C	-6.982564	-0.067968	0.626980	C	-6.428849	-1.110000	-1.209558
H	-7.989762	0.108576	0.985912	H	-6.965405	-1.067136	-2.151862
C	-6.157576	-0.964260	1.278267	C	-7.124281	-1.122232	-0.014787
H	-6.521988	-1.509412	2.143612	H	-8.207809	-1.090190	-0.018436
C	-4.864810	-1.209926	0.833811	C	-6.438487	-1.171976	1.184300
C	-4.758758	1.055369	-2.217620	H	-6.981901	-1.176121	2.123639
H	-4.052000	1.847897	-1.960811	C	-5.050522	-1.215986	1.208900
H	-5.591669	1.499217	-2.764901	C	-4.289719	-1.118987	-2.517412
H	-4.235432	0.357928	-2.876870	H	-3.650404	-0.233555	-2.584553

C	-4.028552	-2.258597	1.496300	H	-4.977066	-1.104635	-3.363831
H	-3.176423	-1.855443	2.053599	H	-3.627286	-1.979955	-2.627724
H	-3.609610	-2.949280	0.760137	C	-4.306969	-1.270610	2.502421
H	-4.627596	-2.834413	2.202803	H	-3.531161	-0.502318	2.555387
C	1.161666	0.148349	2.989218	H	-3.794567	-2.227460	2.629997
C	2.235298	0.882886	3.498714	H	-4.985845	-1.137873	3.345332
C	3.013588	1.187640	2.397317	C	1.328169	1.458701	2.568301
C	0.047389	-0.407697	3.794173	C	2.566612	1.846520	3.097474
H	0.423447	-0.756436	4.757934	C	3.505283	1.319468	2.232365
H	-0.447775	-1.246090	3.304879	C	-0.008736	1.799891	3.107259
H	-0.706299	0.357791	4.008466	H	0.010221	1.817637	4.198795
C	2.457806	1.231920	4.924806	H	-0.771204	1.089302	2.785408
H	3.352565	1.841755	5.054678	H	-0.320353	2.790879	2.763380
H	2.580990	0.340510	5.546717	C	2.780219	2.652833	4.326195
H	1.616576	1.794862	5.339016	H	3.835629	2.885418	4.475545
C	4.291336	1.935539	2.329652	H	2.433109	2.131031	5.223096
H	4.227615	2.781971	1.641798	H	2.241652	3.603712	4.282889
H	5.112274	1.302255	1.985234	C	4.984078	1.398648	2.284807
H	4.555208	2.320072	3.314429	H	5.396405	1.904986	1.409098
C	2.398063	-2.852068	-1.014696	H	5.440304	0.406702	2.328191
C	3.760940	-2.771475	-1.313771	H	5.299822	1.951288	3.169527
C	4.107514	-1.458540	-1.062610	C	1.532348	-3.174668	-0.010763
C	1.563794	-4.070317	-1.118136	C	2.823175	-3.717420	-0.019220
H	0.693325	-4.030126	-0.465945	C	3.670153	-2.627687	-0.018657
H	2.154652	-4.948322	-0.850313	C	0.264524	-3.944359	-0.008033
H	1.207125	-4.221768	-2.141030	H	-0.338377	-3.730963	0.876752

C	4.615479	-3.890022	-1.786951	H	0.482901	-5.012763	-0.009774
H	4.223074	-4.337423	-2.704316	H	-0.343218	-3.729192	-0.889094
H	4.681428	-4.691438	-1.045197	C	3.175829	-5.160934	-0.027106
H	5.633251	-3.558782	-1.996292	H	2.777124	-5.672810	-0.907331
C	5.432718	-0.806713	-1.185636	H	2.783618	-5.680839	0.851311
H	5.406323	0.036406	-1.879685	H	4.256735	-5.306210	-0.031836
H	6.167560	-1.521894	-1.554079	C	5.151819	-2.592808	-0.025104
H	5.787855	-0.424402	-0.225789	H	5.541492	-2.074445	-0.904312
C	0.124949	1.682140	-2.215962	H	5.549850	-3.607210	-0.030201
C	1.006265	2.707432	-2.590689	H	5.549256	-2.080103	0.853957
C	2.135707	2.505360	-1.826531	C	1.313226	1.465950	-2.563411
C	-1.204015	1.452798	-2.824098	C	2.548623	1.858898	-3.095584
H	-1.884868	2.276055	-2.590931	C	3.491536	1.334957	-2.233534
H	-1.672517	0.534119	-2.480732	C	-0.024643	1.797107	-3.106013
H	-1.109804	1.407953	-3.912526	H	-0.311985	2.817023	-2.832271
C	0.729135	3.756446	-3.603771	H	-0.794729	1.125889	-2.724666
H	1.553541	4.465398	-3.691052	H	-0.021428	1.737522	-4.196579
H	-0.170346	4.327737	-3.352610	C	2.752894	2.666198	-4.325033
H	0.561655	3.327298	-4.596198	H	3.806698	2.901189	-4.481750
C	3.411112	3.260284	-1.806673	H	2.212131	3.615758	-4.277863
H	3.336137	4.143873	-2.440109	H	2.400343	2.143941	-5.219597
H	4.245865	2.657129	-2.172790	C	4.969812	1.420307	-2.290222
H	3.671357	3.589963	-0.797529	H	5.280231	1.982743	-3.170655
O	-0.783229	2.525616	1.110509	H	5.429983	0.430726	-2.344784
C	-0.526819	3.864080	0.680032	H	5.382926	1.919830	-1.411002
C	0.836110	4.233961	1.187849	C	-3.378269	3.844577	0.021092

H	-1.311782	4.522118	1.064149	C	-3.398580	5.345071	0.026408
H	-0.573786	3.900631	-0.413876	H	-3.887627	3.436254	0.902204
H	1.103625	5.240563	0.862521	H	-3.881920	3.442349	-0.866120
H	0.874101	4.200475	2.278412	H	-4.426891	5.709006	0.024335
H	1.579087	3.532087	0.799511	H	-2.896740	5.735331	0.912976
H	-1.064955	0.294028	1.709500	H	-2.890846	5.741715	-0.853949

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