Electronic Supplementary Information

2-Imino-2,3-dihydrobenzoxazole – a Useful Platform for Designing Rare- and Alkaline Earth Complexes with Variable Di- and Trianionic O,N,N, Ligands

Ivan V. Basalov,[a] Alexander A. Kissel,[b] Elena N. Nikolaevskaya,[c] Nikolai O. Druzhkov,[a] Anton V. Cherkasov,[a] Jérôme Long, [d] Joulia Larionova ,[d] Georgy K.Fukin,[a] Alexander A. Trifonov[a,b,*]

[a]G. A. Razuvaev Institute of Organometallic Chemistry of Russian Academy of Sciences, 603137, 49 Tropinina str., Nizhny Novgorod, Russia GSP-445, Fax: + 007-831-462-74-97 E-mail: trif@iomc.ras.ru.
[b]A. N. Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, 28 Vavilova str., 119991, Moscow,GSP-1, Russia
[c]N. D. Zelinsky Institute of Organic Chemistry of Russian Academy of Sciences, 47 Leninsky Av., 119991, Moscow, GSP-1, Russia.
[d]Institut Charles Gerhardt, Equipe Ingénierie Moléculaire et Nano-Objets, Université de Montpellier, ENSCM, CNRS. Place Eugène Bataillon, 34095 Montpellier Cedex 5, France

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Table S1. Crystal data and structure refinement details for complexes **1-3, 5**.

	1	**2**	**3**	**5**
Empirical formula	$C_{40}H_{71}N_3O_3Si_2Yb$, $1½C_4H_8O$	$C_{68}H_{100}Ca_2N_4O_4$, C_4H_8O	$C_{76}H_{116}CaN_4Na_2O_6$, C_6H_{14}	$C_{42}H_{73}N_2O_5SiY$, $½C_6H_{14}$, $½C_4H_8O$
Formula weight	979.37	1189.78	1353.95	882.16
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P2₁/n*	*C2*	*C2/c*	*P2₁/c*
Unit cell dimensions	a = 15.1288(18)Å b = 15.8035(18)Å c = 22.479(3)Å α = 90° β =101.070(2)° γ = 90°	a = 19.1393(14)Å b = 17.1302(13)Å c = 13.5419(10)Å α = 90° β =130.5560(10)° γ = 90°	a = 23.3970(13)Å b = 17.8742(10)Å c = 20.0635(11)Å α = 90° β =110.4960(10)° γ = 90°	a = 14.7864(2)Å b = 18.1974(2)Å c = 18.7593(3)Å α = 90° β =98.6680(14)° γ = 90°
V, Å^3	5274.5(11)	3373.3(4)	7859.5(8)	4989.99(12)
Z	4	2	4	4
d_{calc}, g/cm^3	1.233	1.171	1.144	1.174
μ, mm^{-1}	1.858	0.220	0.143	1.236
F_{000}	2056	1296	2960	1908
Crystal dimensions, mm	0.25×0.20×0.05	0.28×0.20×0.10	0.41×0.30×0.19	0.30×0.20×0.20
ϑ range for data collection, °	1.88-27.19	2.80-29.90	2.52-28.82	2.94-30.03
HKL indicies	-19<=h<=19 -20<=k<=19 -23<=l<=28	-26<=h<=26 -23<=k<=23 -18<=l<=18	-31<=h<=31 -24<=k<=24 -26<=l<=27	-20<=h<=20 -25<=k<=25 -26<=l<=26
Reflns collected	36244	20310	50191	103537
Independent reflns (R_{int})	11681 (0.0686)	9632 (0.0290)	10182 (0.0322)	14579 (0.0934)
Completeness to ϑ, %	99.4	99.7	99.8	99.9
Data / restraints / parameters	11681 / 180 / 571	9632 / 207 / 537	10182 / 63 / 488	14579 / 235 / 618
$S(F^2)$	1.000	1.060	1.011	1.034
Final *R* indices ($I>2\sigma(I)$)	R_1 = 0.0480 wR_2 = 0.1068	R_1 = 0.0639 wR_2 = 0.1601	R_1 = 0.0473 wR_2 = 0.1216	R_1 = 0.0556 wR_2 = 0.1118
R indices (all data)	R_1 = 0.0923 wR_2 = 0.1263	R_1 = 0.0711 wR_2 = 0.1652	R_1 = 0.0602 wR_2 = 0.1312	R_1 = 0.0881 wR_2 = 0.1240
Flack parameter		0.08(5)		
Largest diff peak and hole, e/Å^3	2.16 / -0.97	0.62 / -0.50	0.54 / -0.23	1.01 / -0.60

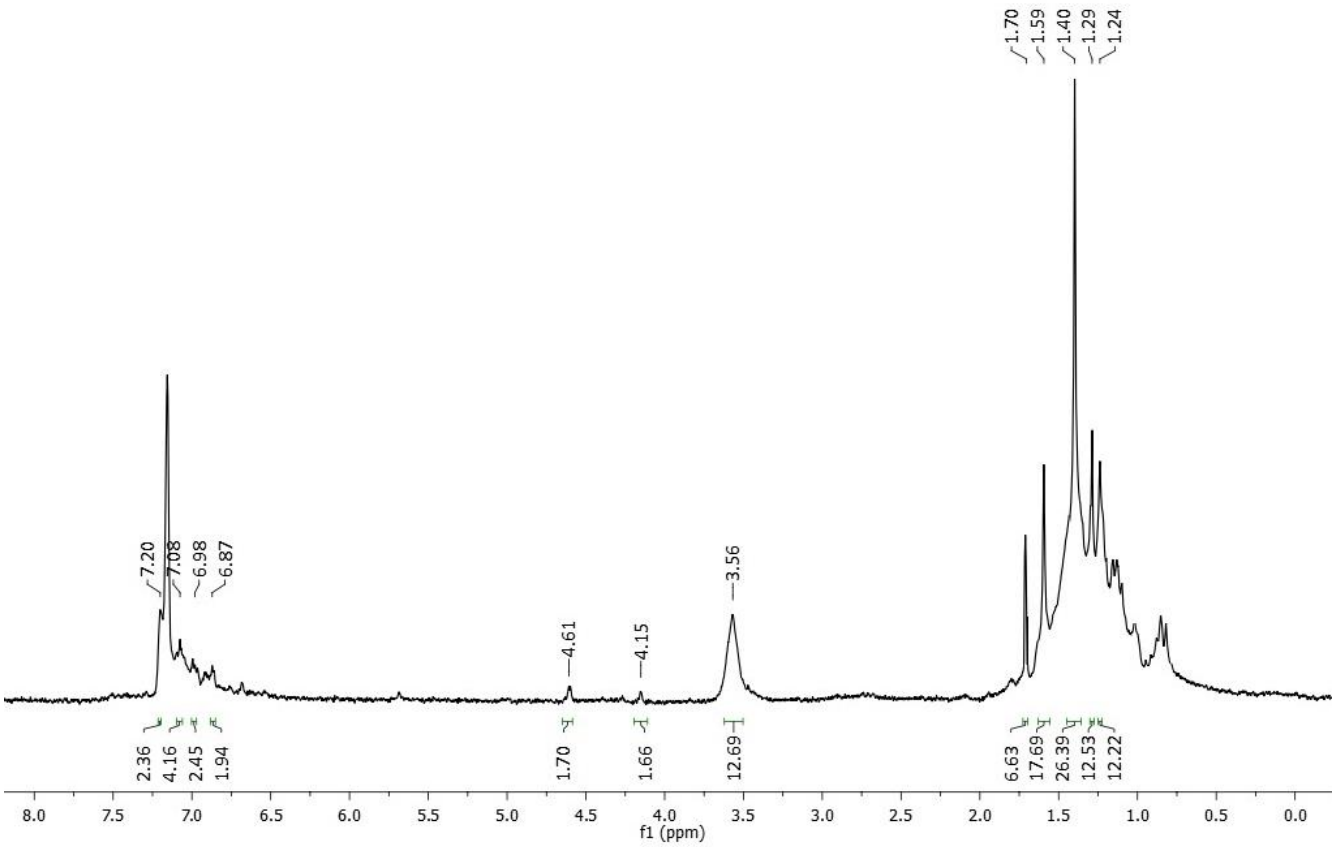

Figure S1. ^{1}H NMR spectrum (400 MHz, C_6D_6) of **2**.

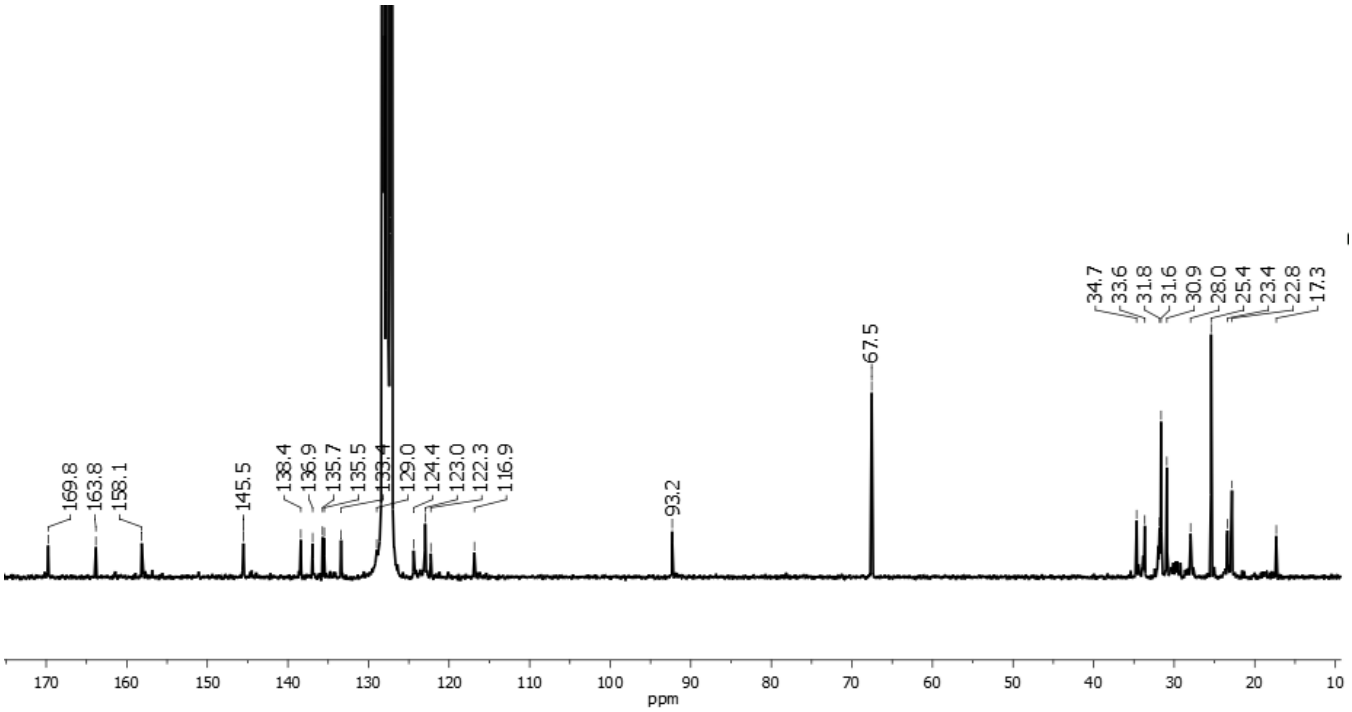

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, C_6D_6) of **2.**

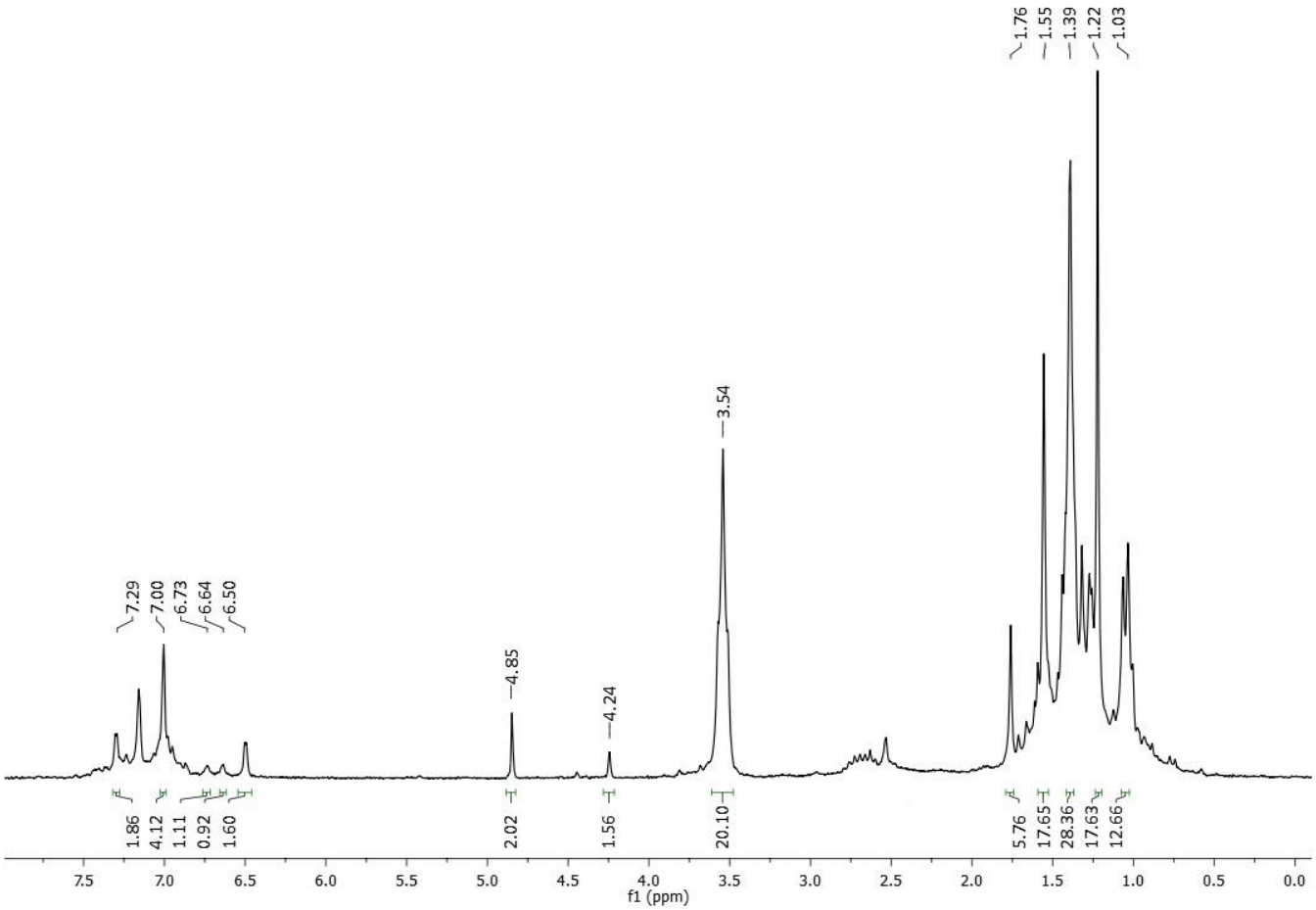

Figure S3. ^{1}H NMR spectrum (400 MHz, C_6D_6) of **3**.

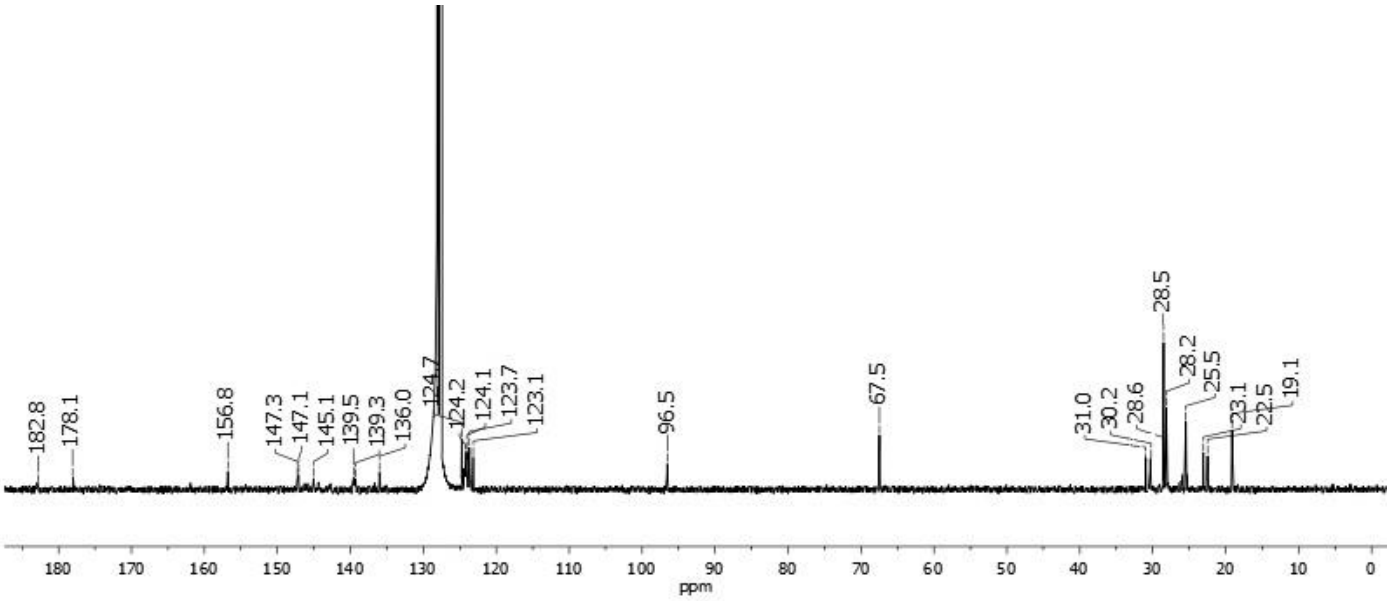

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, C_6D_6) of **3.**

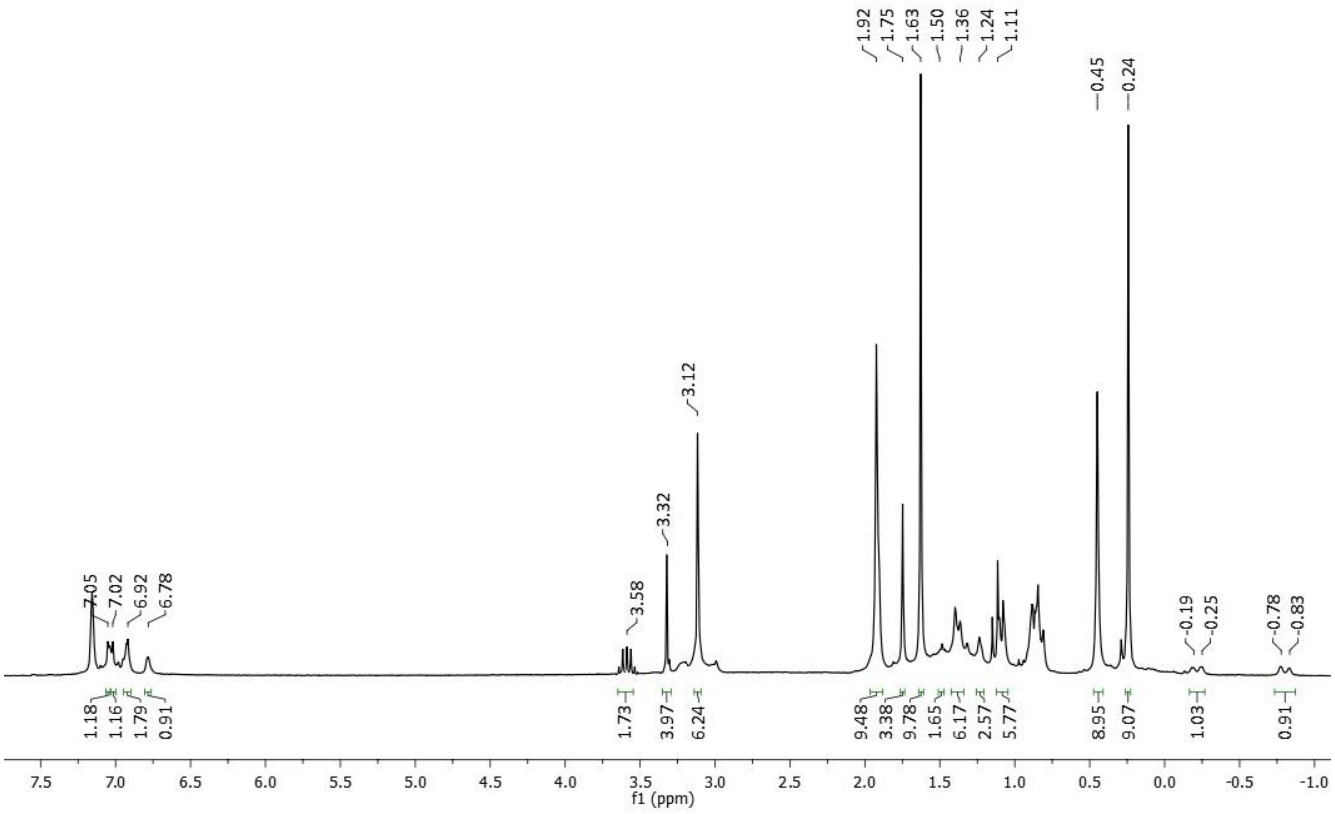

Figure S5. ^{1}H NMR spectrum (400 MHz, C_6D_6) of **4**.

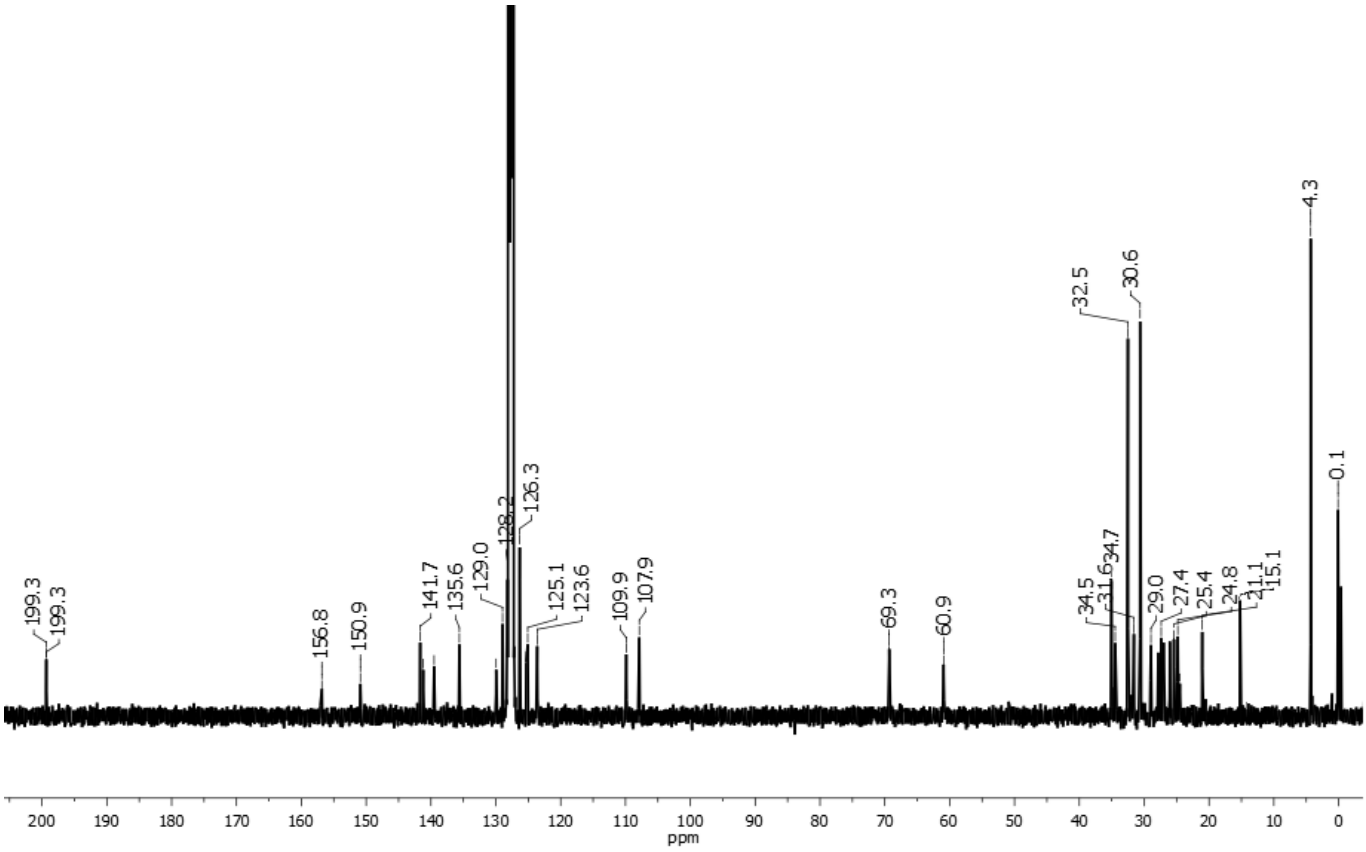

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, C_6D_6) of **4**.

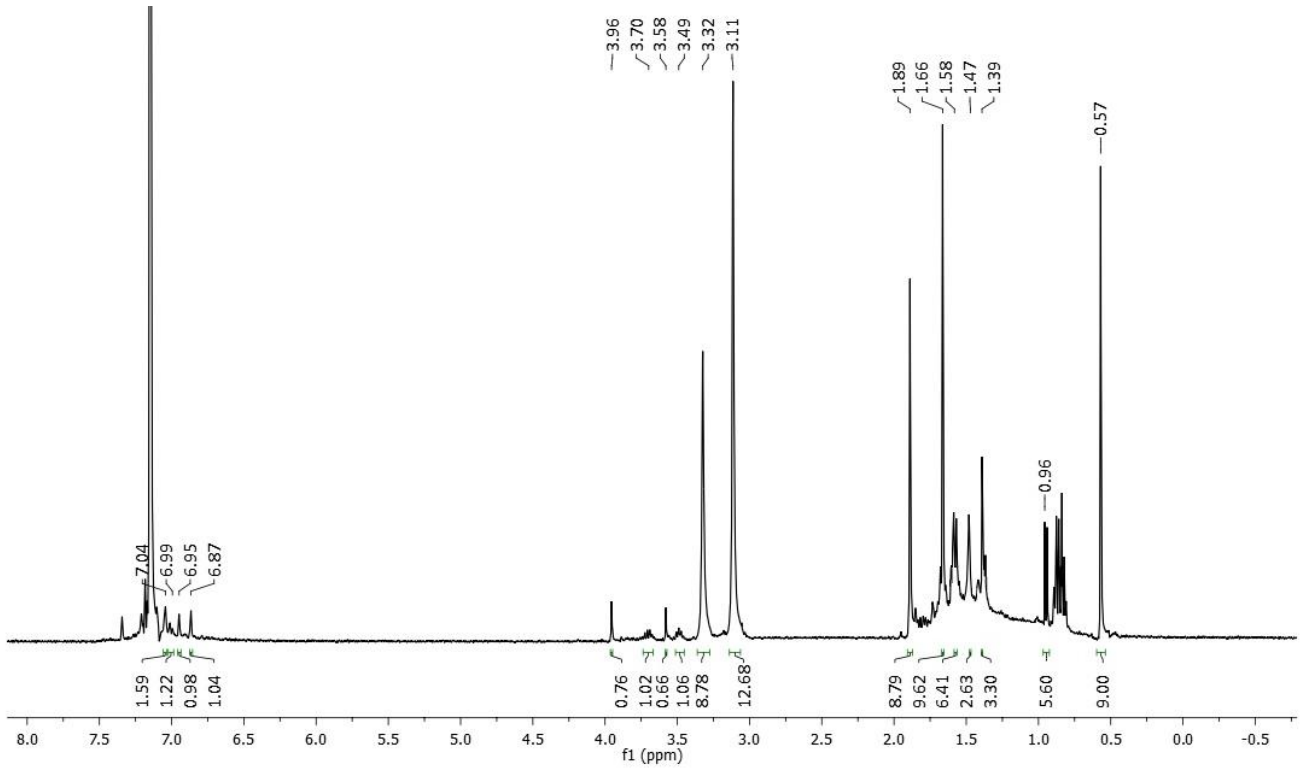

Figure S7. ^{1}H NMR spectrum (400 MHz, C_6D_6) of **5**.

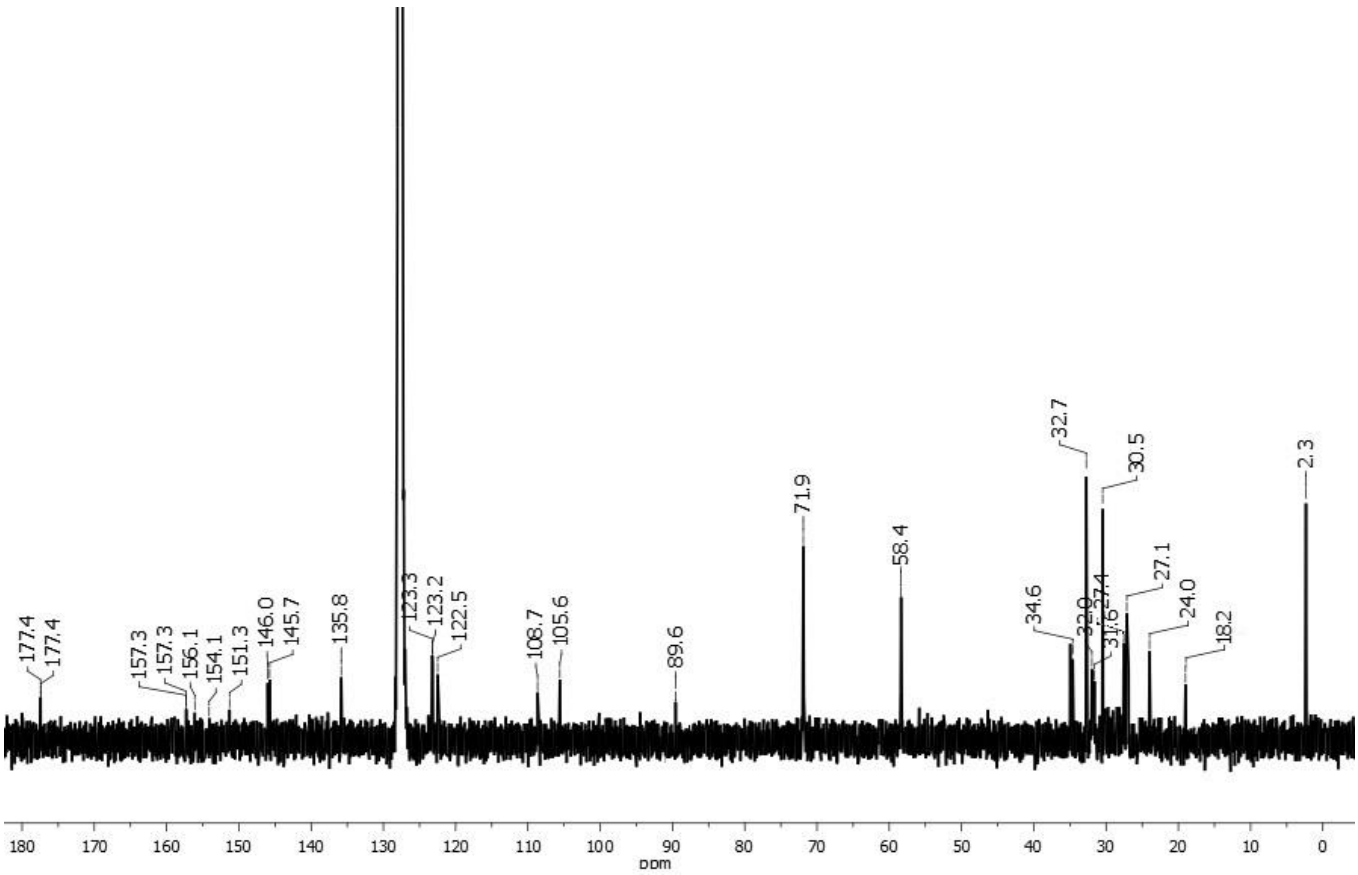

Figure S8. ^{13}C{^{1}H} NMR spectrum (101 MHz, C_6D_6) of **5**