Supporting Information

for

LUMINESCENT INDIUM COMPLEXES WITH ONN-DONOR SCHIFF BASES: SYNTHESIS, STRUCTURE, AND DFT INVESTIGATION

Irina V. Ershova[a,*], Svetlana V. Baryshnikova[a], Maxim V. Arsenyev[a], Alexey A. Belikov[a], Ilya A. Yakushev[b], Pavel V. Dorovatovskii[c], Vasily A. Ilichev[a], Sergey Yu. Ketkov[a], Alexandr V. Piskunov[a,*]

[a]*G. A. Razuvaev Institute of Organometallic Chemistry of Russian Academy of Sciences, 49 Tropinina str., 603950 Nizhny Novgorod, Russia*

[b]*N. S. Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Leninskii prosp. 31, 119991 Moscow, Russia*

[c]*National Research Center 'Kurchatov Institute', Kurchatov sq. 1, 123182 Moscow, Russia*

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*Corresponding author: E-mail address: irina@iomc.ras.ru (I.V. Ershova), pial@iomc.ras.ru (A.V. Piskunov)

Table S1. Crystallographic data and structure refinement details for **1-4**

Compound	**1**	**2**	**3**	**4**
Empirical formula	$C_{28}H_{30}In_2N_4O_2$	$C_{30}H_{34}In_2N_4O_2$	$C_{28}H_{28}Cl_2In_2N_4O_2$	$C_{28}H_{28}In_2N_6O_6$
Formula weight	684.20	712.25	753.08	774.20
Temperature [K]	100(2)	100(2)	100(2)	100(2)
Wavelength [Å]	0.75268	0.71073	0.71073	0.75268
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	*C*2/*c*	$P2_1/n$	$P2_1/n$	*P*-1
Unit cell dimensions				
a [Å]	21.051(6)	8.6219(5)	8.5866(2)	7.9004(19)
b [Å]	10.1465(9)	17.4483(11)	17.1574(5)	8.4003(17)
c [Å]	13.0494(9)	9.7888(6)	9.9567(3)	11.382(3)
α [˚]	90	90	90	77.261(5)
β [˚]	111.090(9)	102.362(2)	102.3870(10)	82.036(18)
γ [˚]	90	90	90	89.638(19)
V [Å^3]	2600.6(8)	1438.46(15)	1432.71(7)	729.4(3)
Z	4	2	2	1
d_{calc} [g cm^{-3}]	1.748	1.644	1.746	1.762
μ [mm^{-1}]	2.094	1.636	1.829	1.893
F_{000}	1360	712	744	384
Crystal dimensions [mm^3]	0.09 × 0.05 × 0.03	0.15 × 0.14 × 0.12	0.24 × 0.20 × 0.04	0.06 × 0.05 × 0.02
θ range for data collection [˚]	2.393–26.644	2.335–30.532	2.374–30.503	1.962–26.960
Reflections collected	2277	21821	23889	5470
Independent reflections (R_{int})	2277 (R_{int} = 0.0268)	4391 (R_{int} = 0.0563)	4384 (R_{int} = 0.0333)	2549 (R_{int} = 0.0447)
Completeness to θ [%]	99.0	100.0	100.0	95.5
Data/restraints/parameters	2277 / 0 / 166	4391 / 0 / 175	4384 / 0 / 174	2549 / 0 / 192
Final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0503 wR_2 = 0.1394	R_1 = 0.0332 wR_2 = 0.0571	R_1 = 0.0200 wR_2 = 0.0467	R_1 = 0.0378 wR_2 = 0.0888
Final *R* indices (all data)	R_1 = 0.0566 wR_2 = 0.1440	R_1 = 0.0515 wR_2 = 0.0635	R_1 = 0.0256 wR_2 = 0.0484	R_1 = 0.0458 wR_2 = 0.0924
$S(F^2)$	1.096	1.038	1.066	1.045
Largest diff. peak and hole [e Å^{-3}]	1.562 / -1.352	0.618 / -0.676	0.464 / -0.395	1.325 / -1.169

Table S2. Selected Bond Lengths (Å) and Angles (º) in **1-4**

	1	**2**	**3**	**4**
In(1)-O(1)	2.195(4)	2.1969(17)	2.2004(11)	2.232(4)
In(1)-N(1)	2.414(5)	2.400(2)	2.3988(13)	2.383(4)
In(1)-N(2)	2.736(5)	2.697(2)	2.6725(14)	2.591(4)
In(1)-O(1A)	2.500(4)	2.5112(17)	2.5404(11)	2.657(3)
C(1)-In(1)-C(2)	143.5(2)	144.89(11)	145.14(8)	148.2(2)
C(1)-In(1)-O(1)	103.45(19)	106.04(9)	104.80(6)	102.57(18)
C(2)-In(1)-O(1)	108.3(2)	103.30(10)	104.04(7)	98.64(19)
C(1)-In(1)-N(1)	103.16(19)	95.11(9)	95.08(6)	106.83(17)
C(2)-In(1)-N(1)	103.9(2)	112.36(9)	112.57(6)	102.38(17)
O(1)-In(1)-N(1)	70.98(15)	71.37(6)	71.12(4)	70.80(13)
C(1)-In(1)-O(1A)	87.56(19)	84.78(8)	84.81(6)	83.12(16)
C(2)-In(1)-O(1A)	87.8(2)	87.87(9)	87.68(6)	82.71(16)
O(1)-In(1)-O(1A)	68.22(15)	69.47(7)	68.89(5)	68.96(13)
N(1)-In(1)-O(1A)	139.19(15)	139.11(6)	138.51(4)	139.74(13)
C(1)-In(1)-N(2)	84.6(2)	84.69(9)	85.14(6)	91.11(17)
C(2)-In(1)-N(2)	85.4(2)	87.86(9)	87.85(6)	89.32(17)
O(1)-In(1)-N(2)	135.31(15)	135.33(6)	135.52(4)	136.91(13)
N(1)-In(1)-N(2)	64.41(16)	64.45(7)	64.80(4)	66.13(14)
O(1A)-In(1)-N(2)	156.39(13)	155.07(6)	155.43(4)	154.02(13)
In(1)-O(1)-In(1A)	111.78(15)	110.53(7)	111.11(5)	111.04(13)

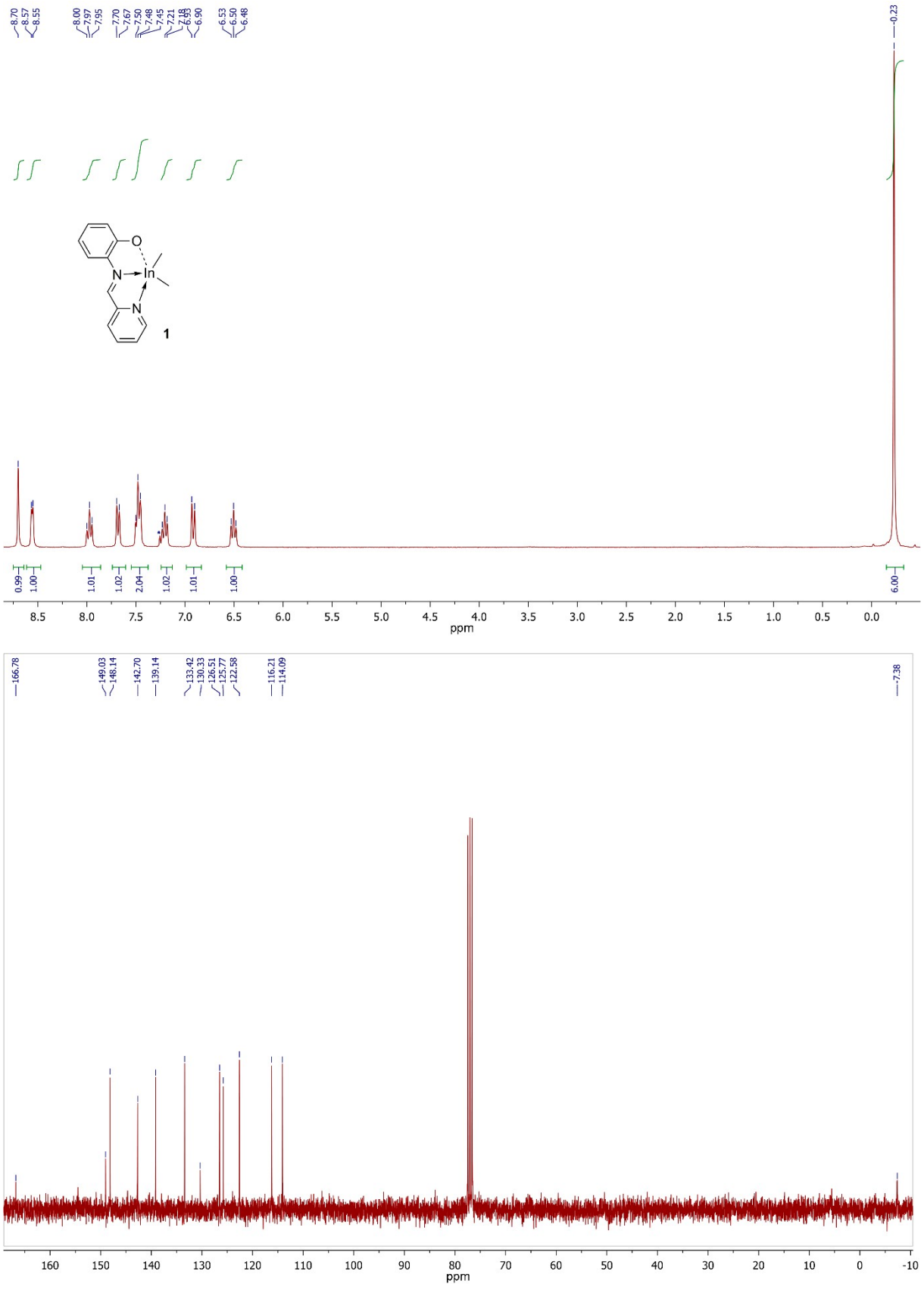


Fig. S1. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **1** (*from residual $CHCl_3$ in $CDCl_3$).

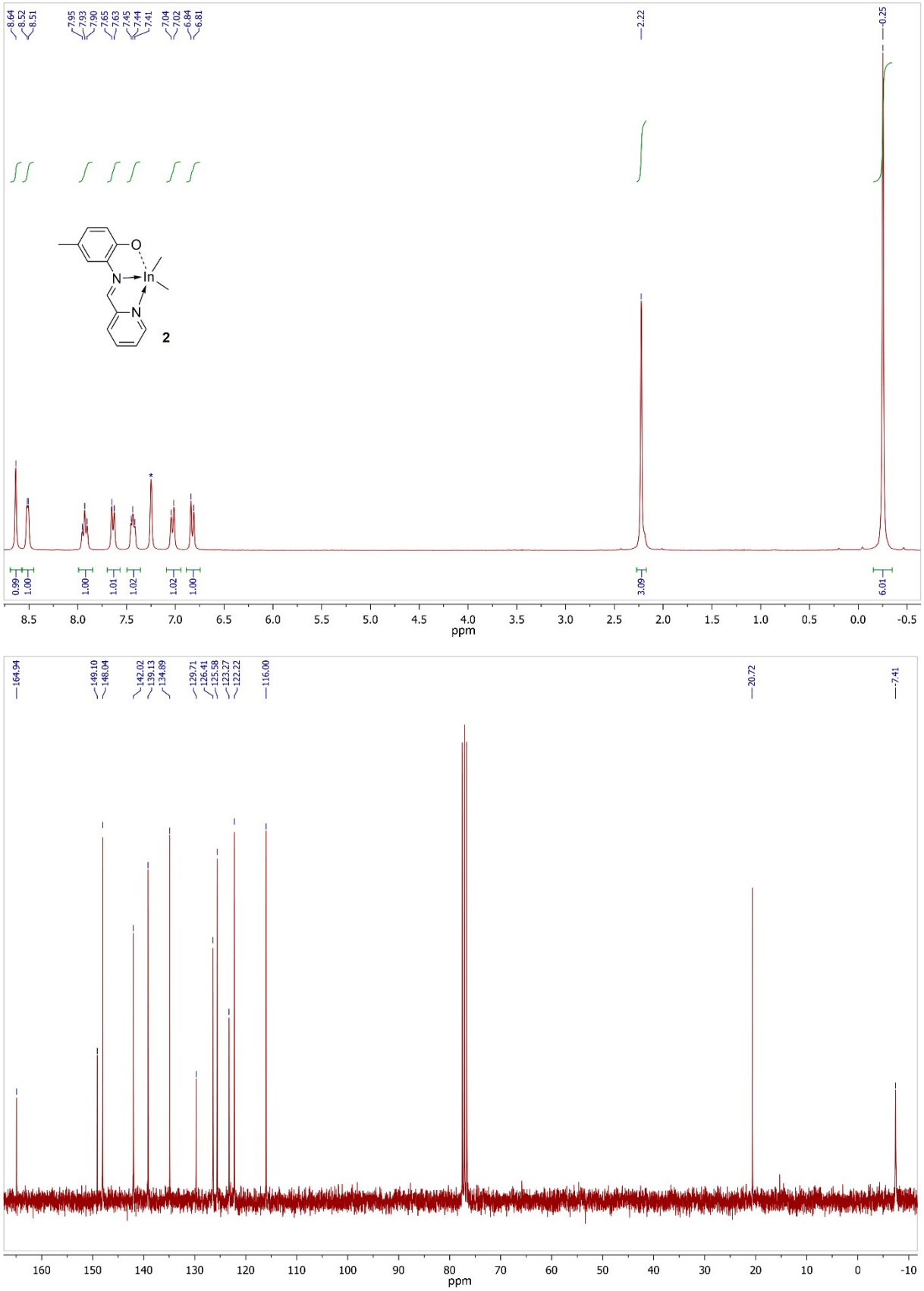


Fig. S2. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **2** (*from residual $CHCl_3$ in $CDCl_3$).

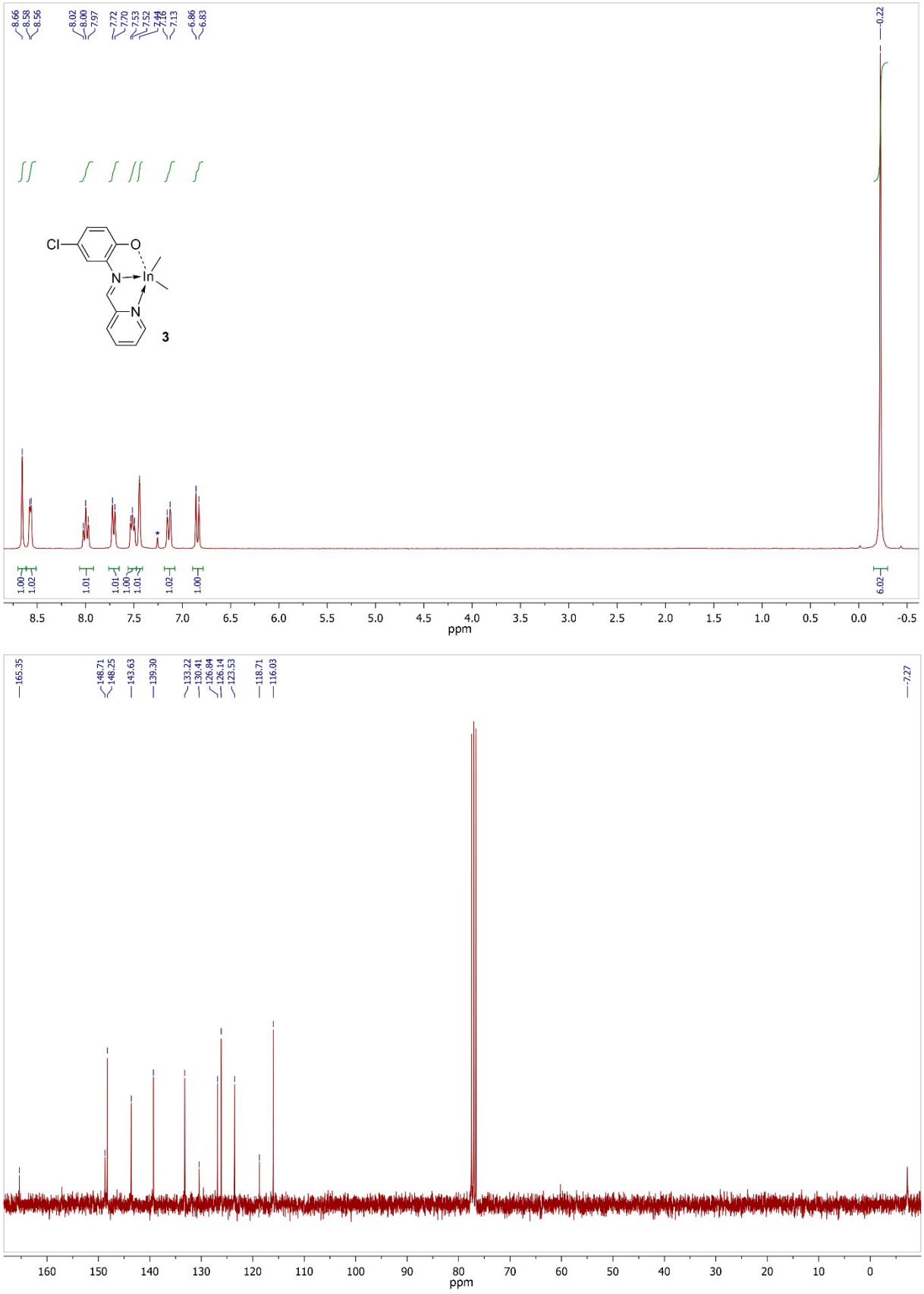


Fig. S3. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **3** (*from residual $CHCl_3$ in $CDCl_3$).

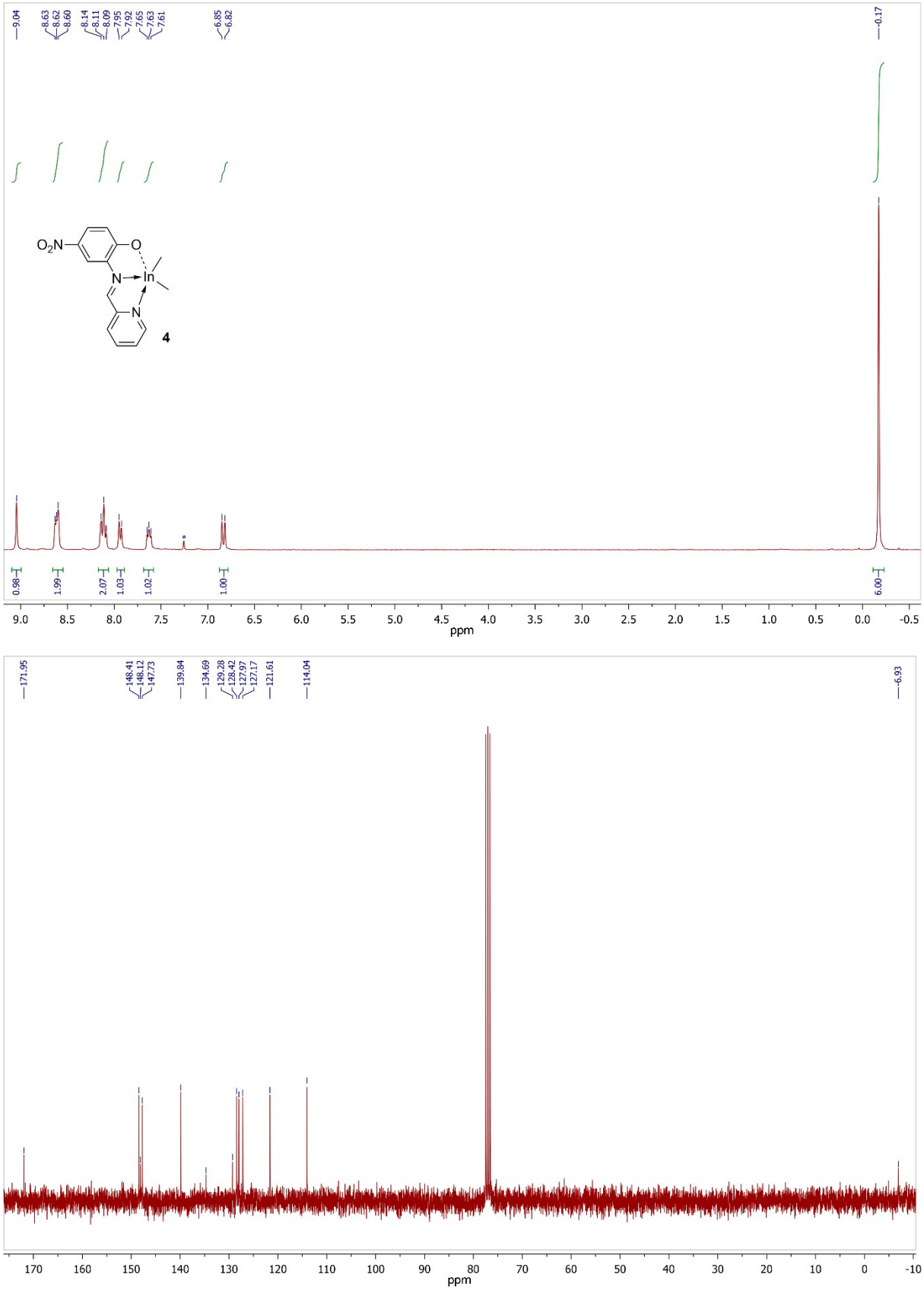


Fig. S4. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4** (*from residual $CHCl_3$ in $CDCl_3$).

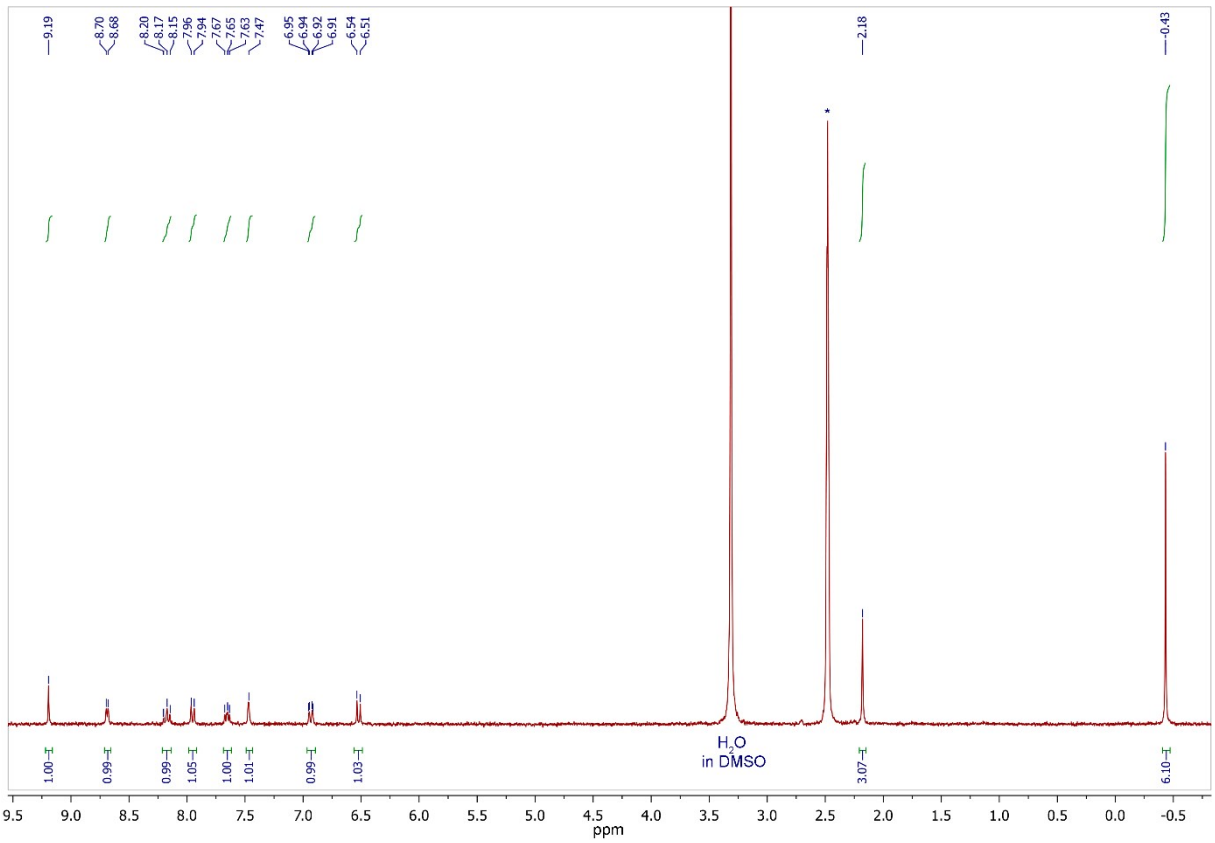


Fig. S5. ^{1}H NMR spectrum of **2** (*from residual DMSO in DMSO-d_6).

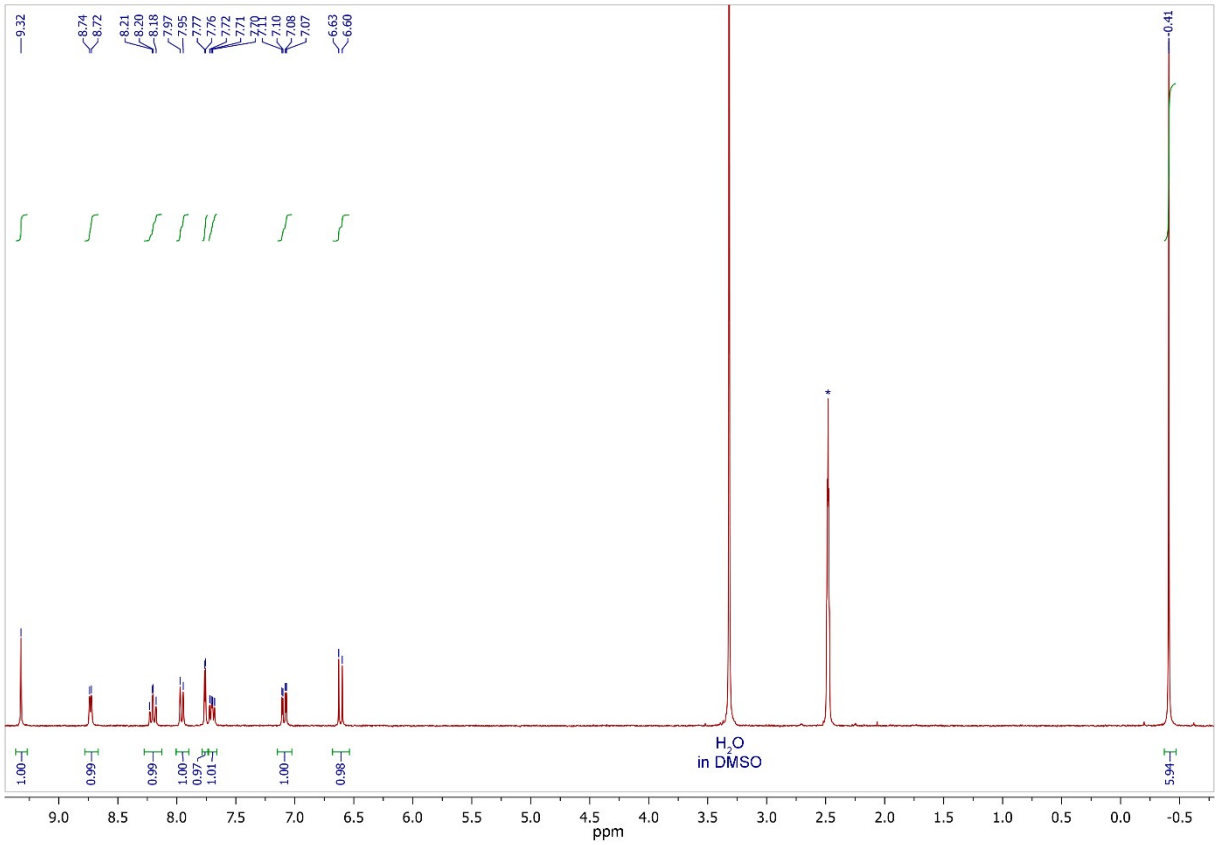


Fig. S6. ^{1}H NMR spectrum of **3** (*from residual DMSO in DMSO-d_6).

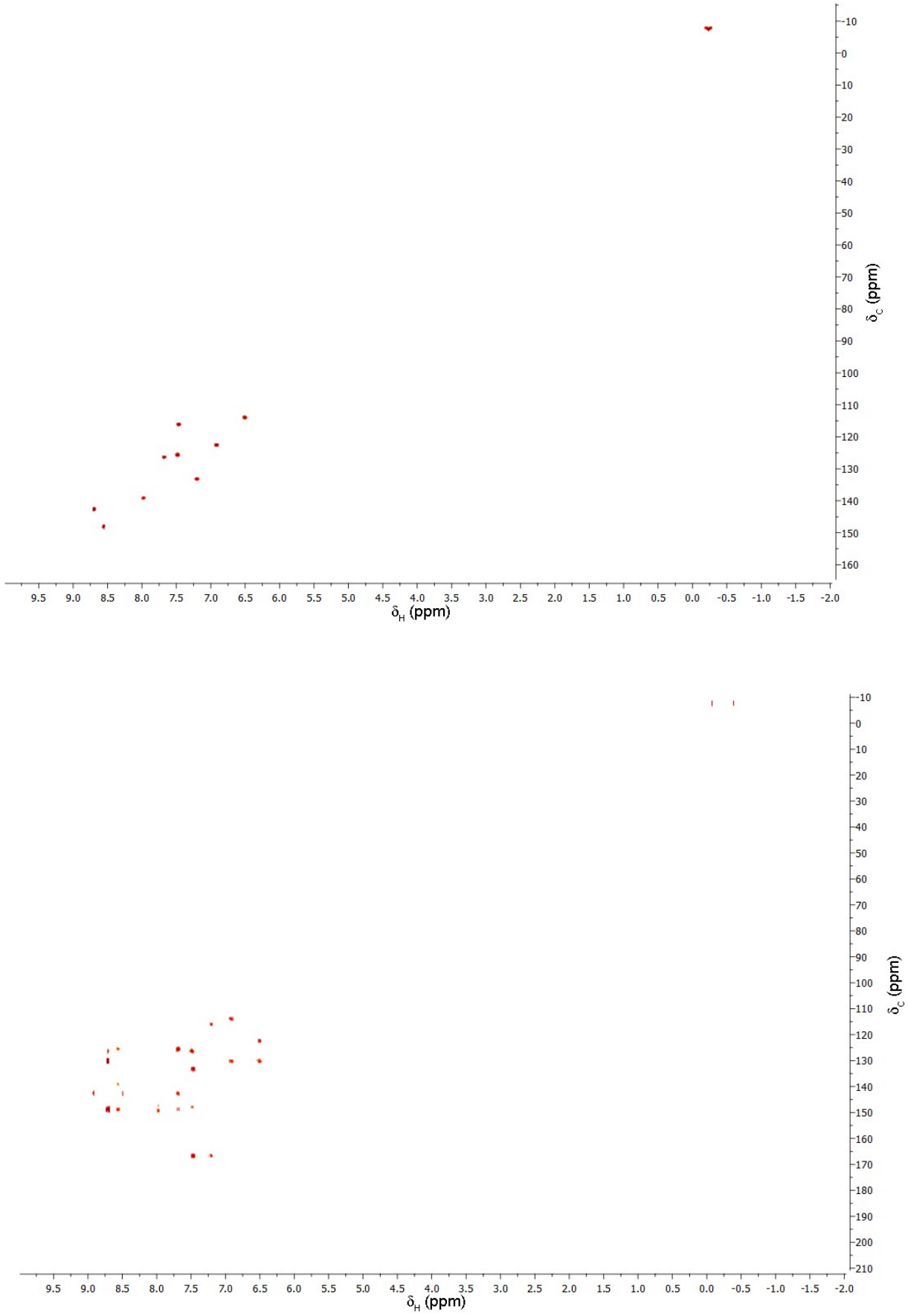


Fig. S7. HSQC (top) and HMBC (bottom) 2D-NMR spectra of **1**

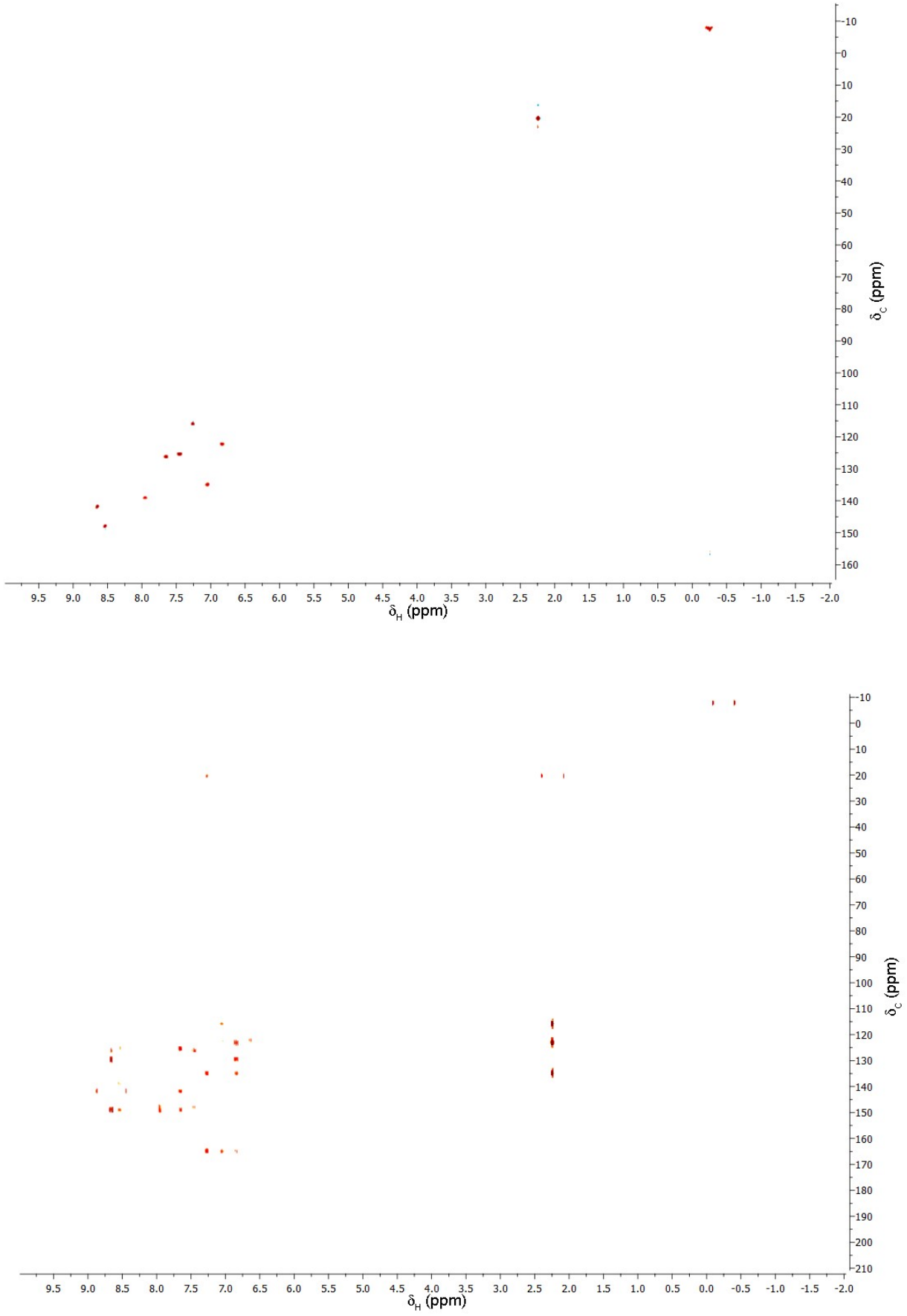


Fig. S8. HSQC (top) and HMBC (bottom) 2D-NMR spectra of **2**

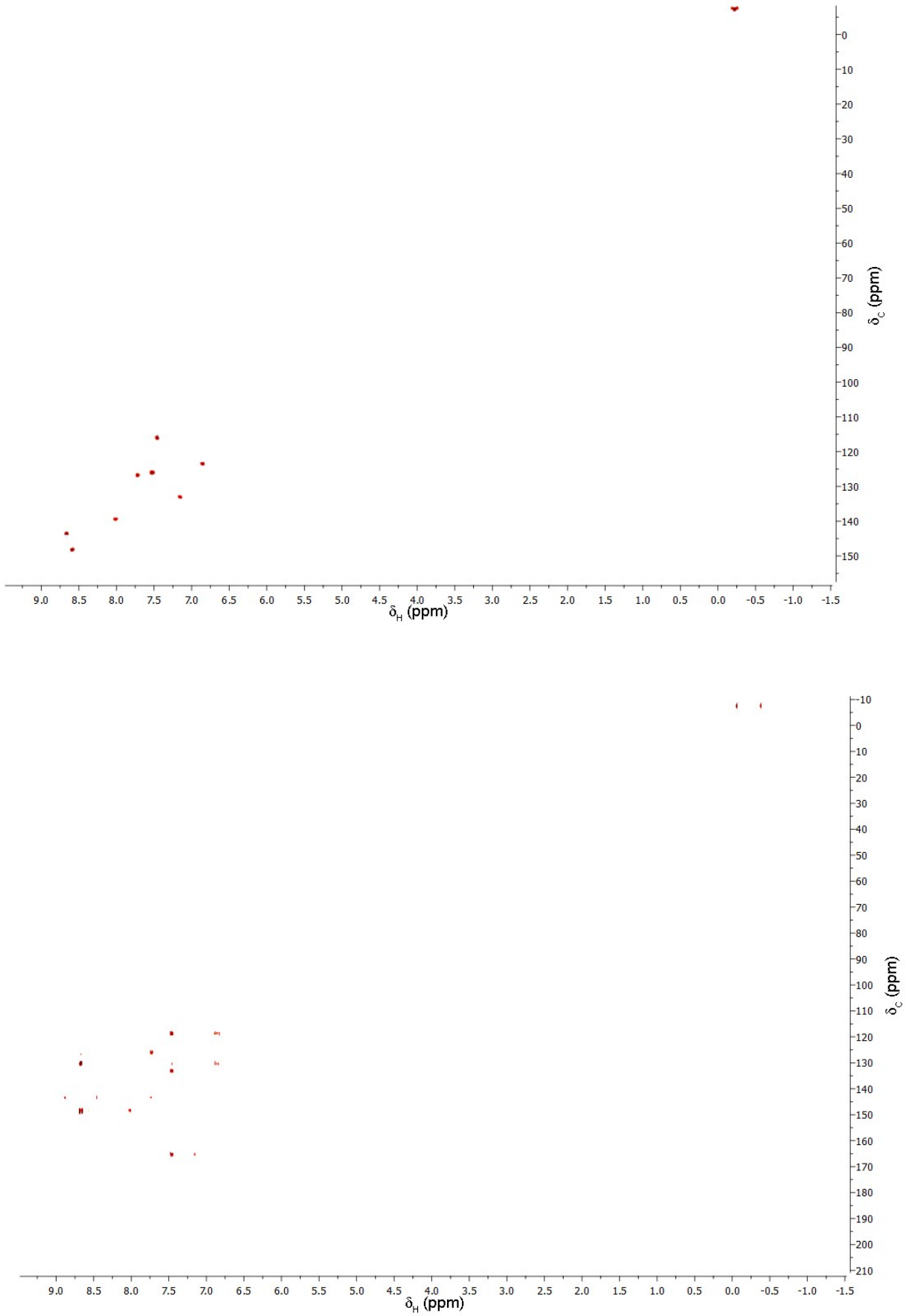


Fig. S9. HSQC (top) and HMBC (bottom) 2D-NMR spectra of **3**

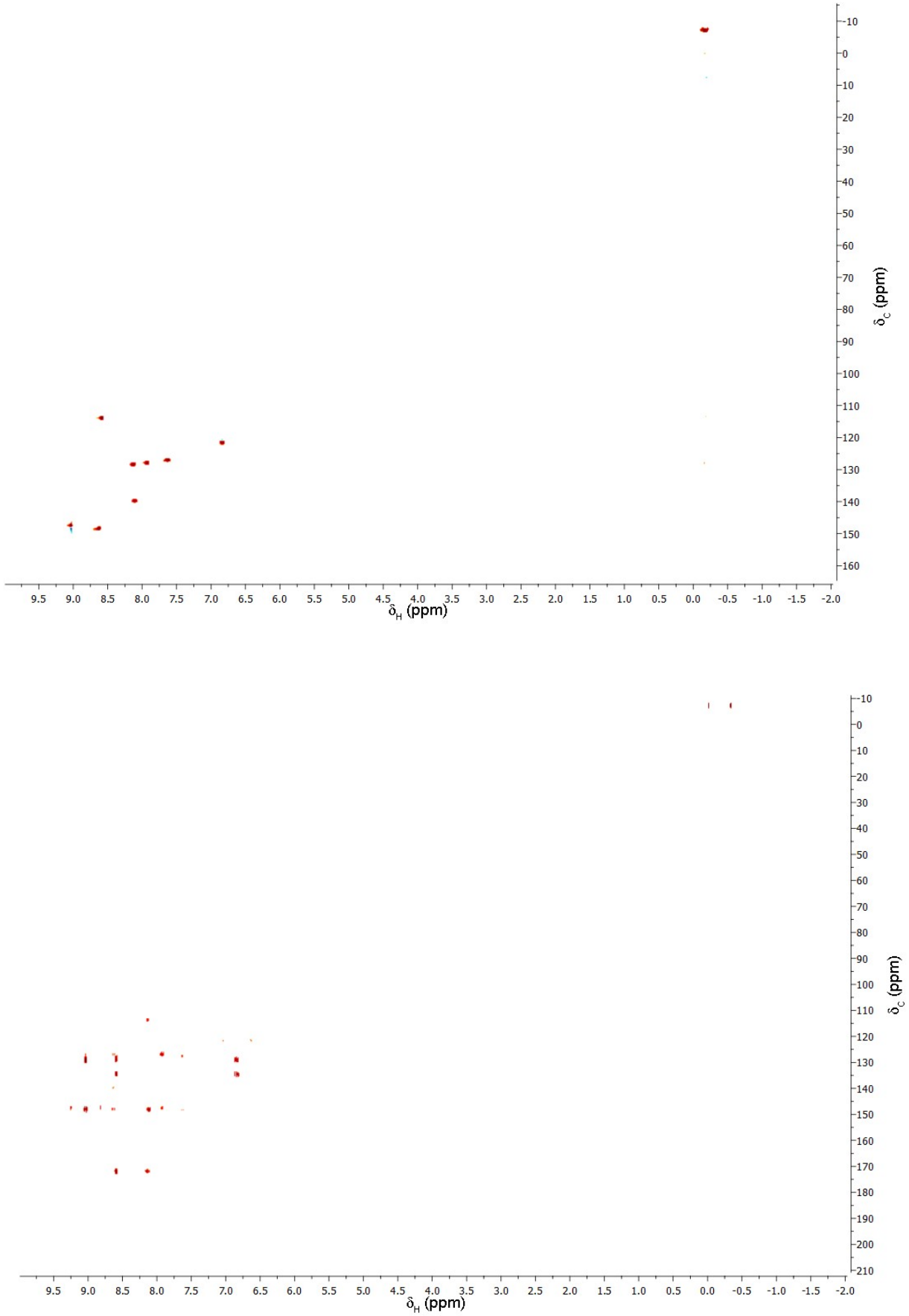


Fig. S10. HSQC (top) and HMBC (bottom) 2D-NMR spectra of **4**

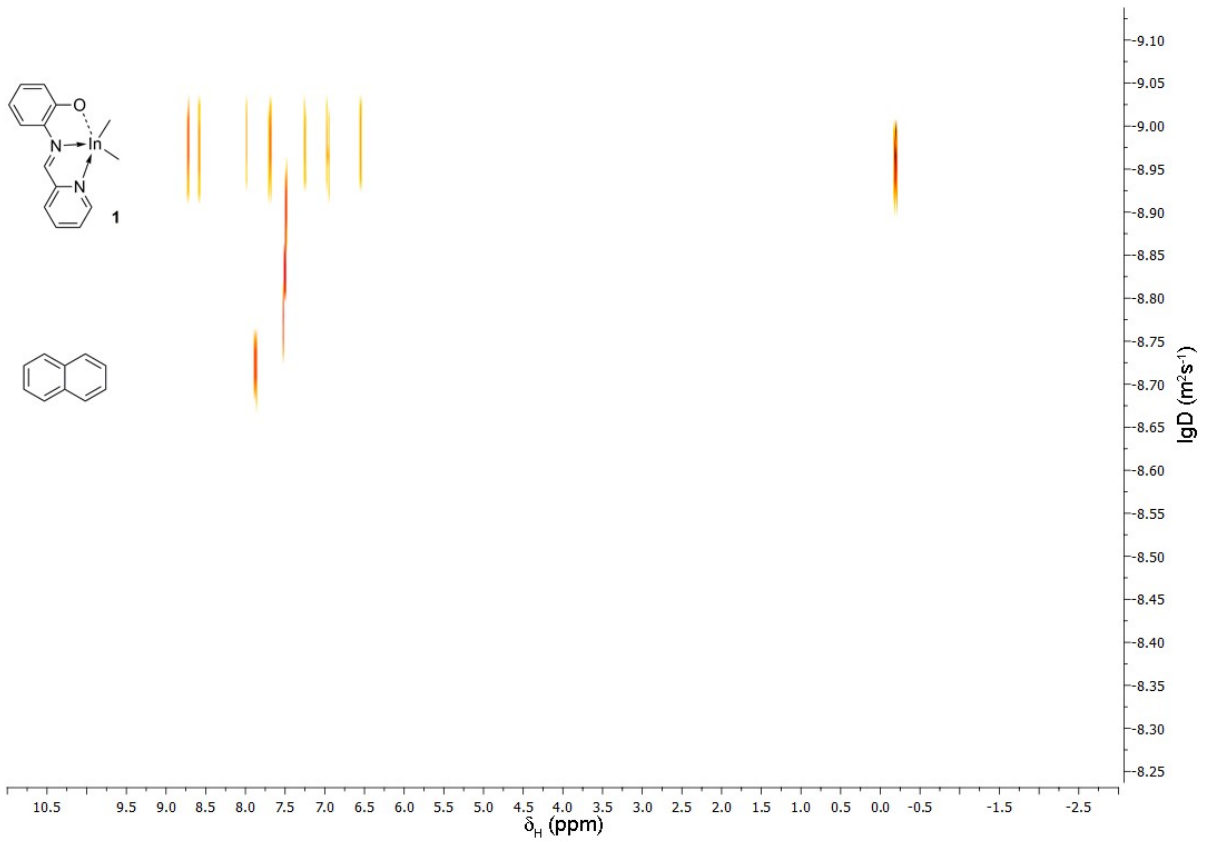


Fig. S11. DOSY spectrum of **1**.

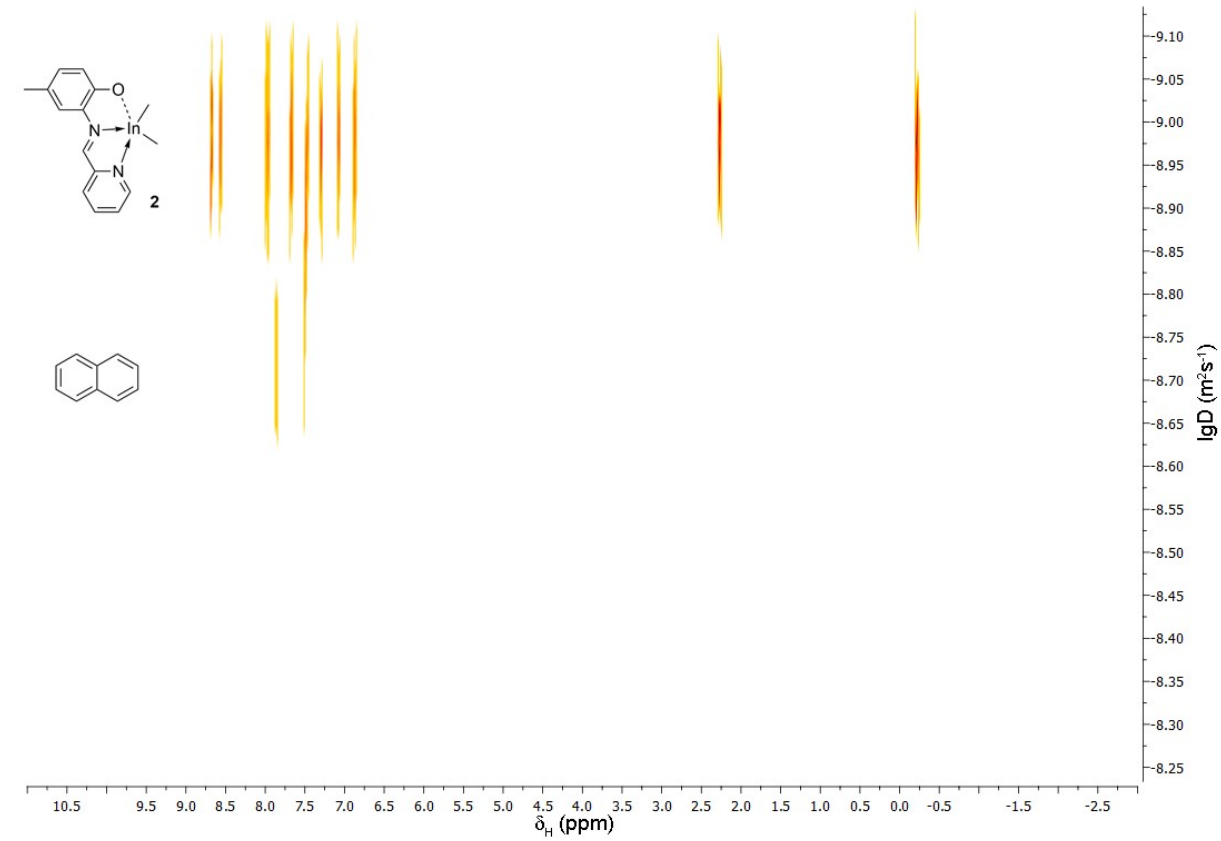


Fig. S12. DOSY spectrum of **2**.

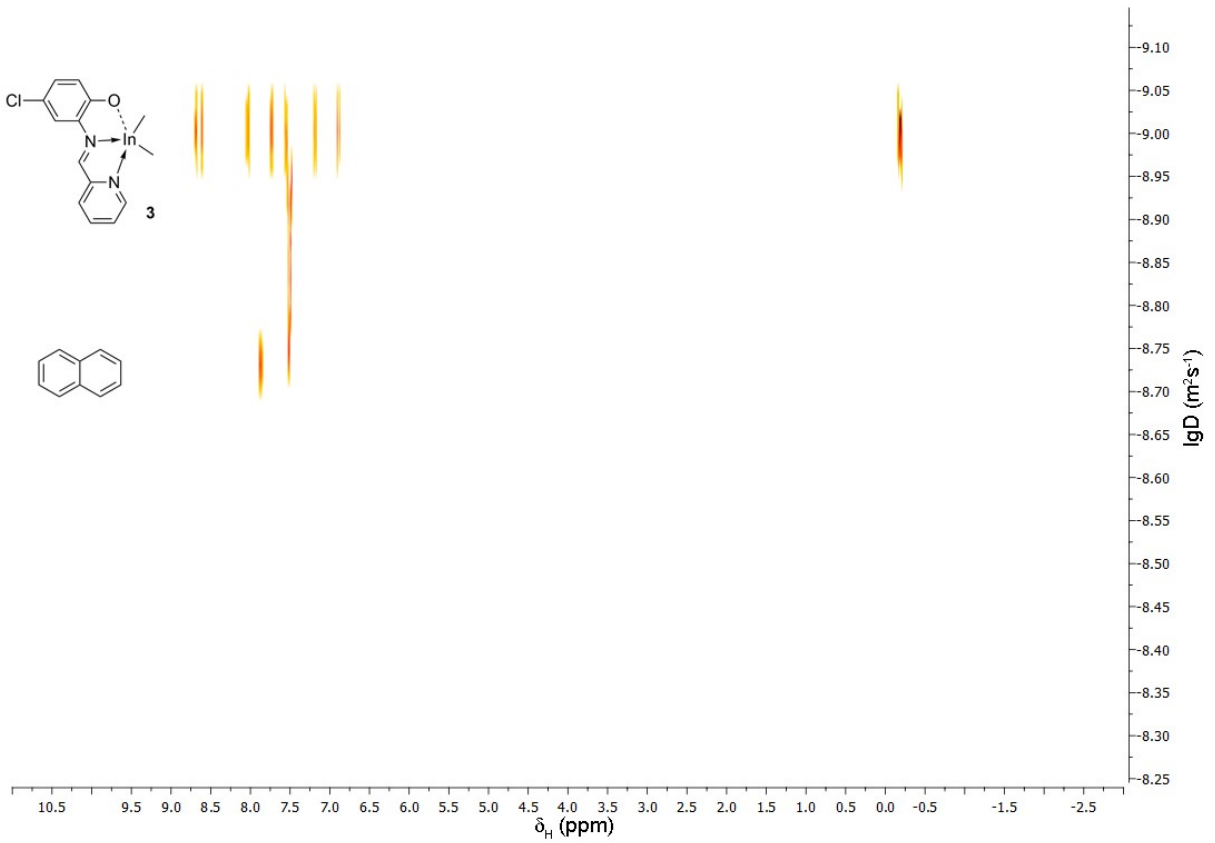


Fig. S13. DOSY spectrum of **3**.

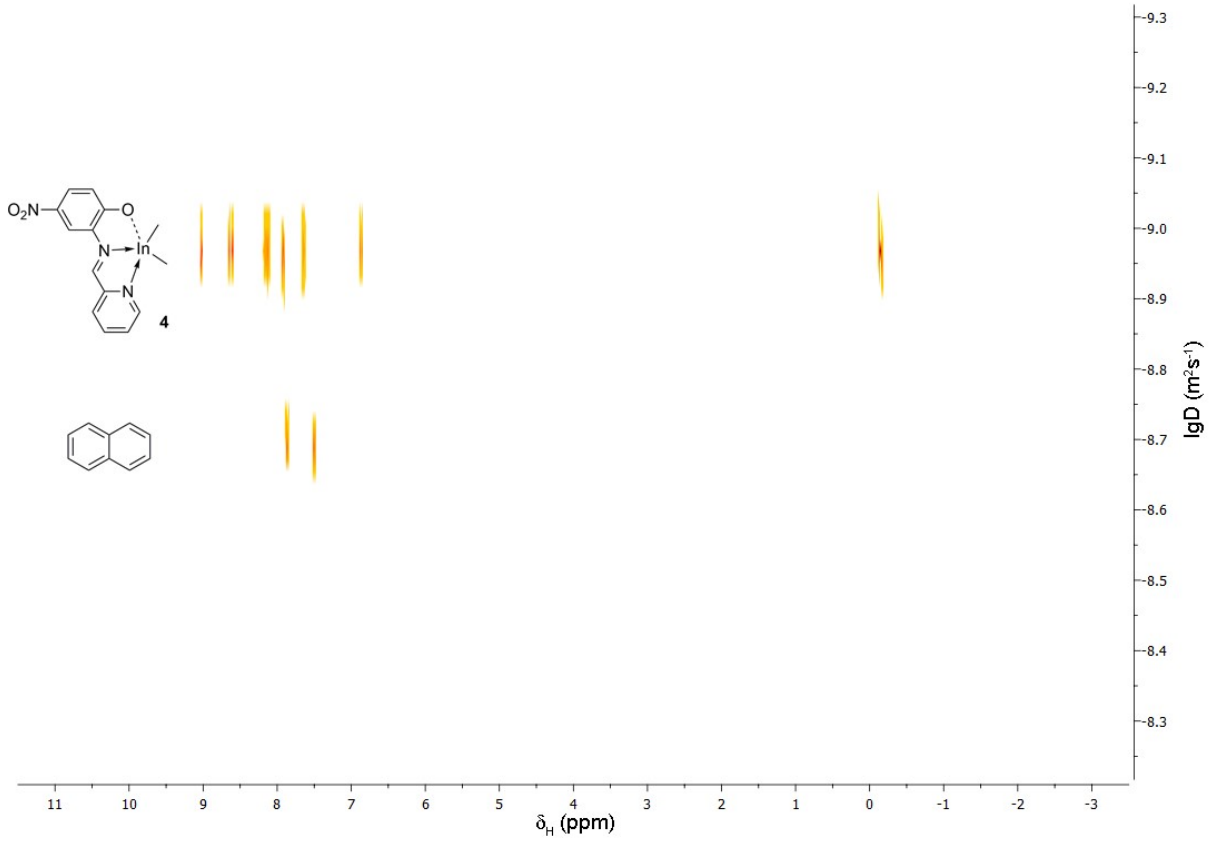
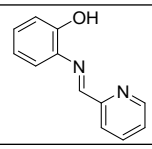
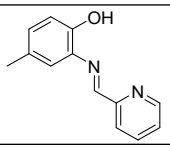
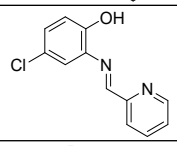
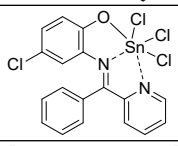
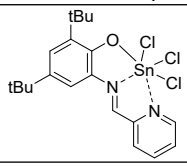
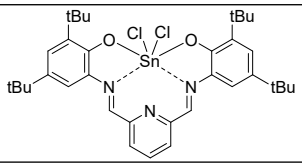
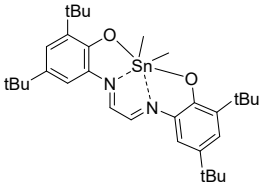
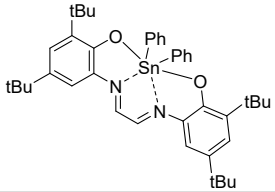
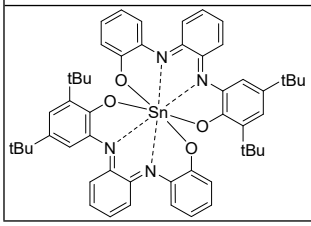
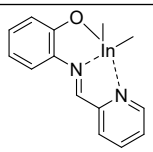
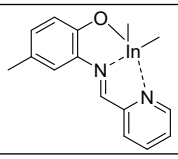
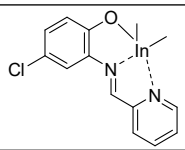
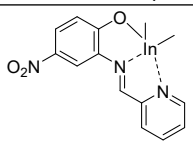
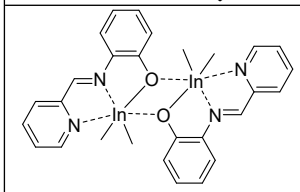
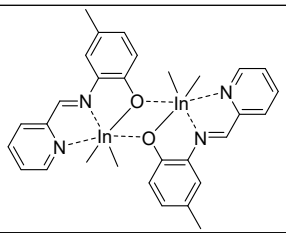
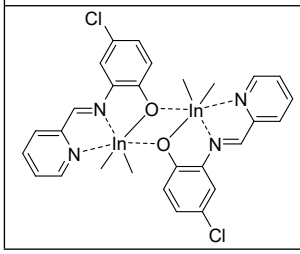
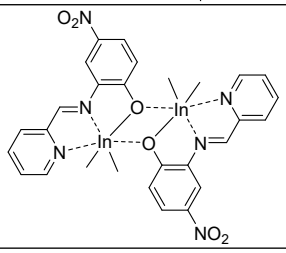


Fig. S14. DOSY spectrum of **4**.

Table S3. Results of measurements of diffusion coefficient (D).

Molecule	M_w	lgM_w	-lgD	ref.	Molecule	M_w	lgM_w	-lgD	ref.
	198.23	2.3	8.95	[1]		212.25	2.33	8.99	[1]
	232.67	2.37	8.97	[2]		532.82	2.73	9.12	[3]
	534.49	2.73	9.14	[3]		729.37	2.86	9.23	[4]
	611.46	2.79	9.18	[5]		735.6	2.87	9.18	[5]
	919.75	2.96	9.32	[6]					

This work

Molecule	M_w	lgM_w	-lgD	Molecule	M_w	lgM_w	-lgD
	342.11	2.53	9.03		356.13	2.55	9.05
	376.55	2.58	9.05		387.10	2.59	9.06
	684.22	2.84	9.03		712.26	2.85	9.05
	753.1	2.88	9.05		774.2	2.89	9.06

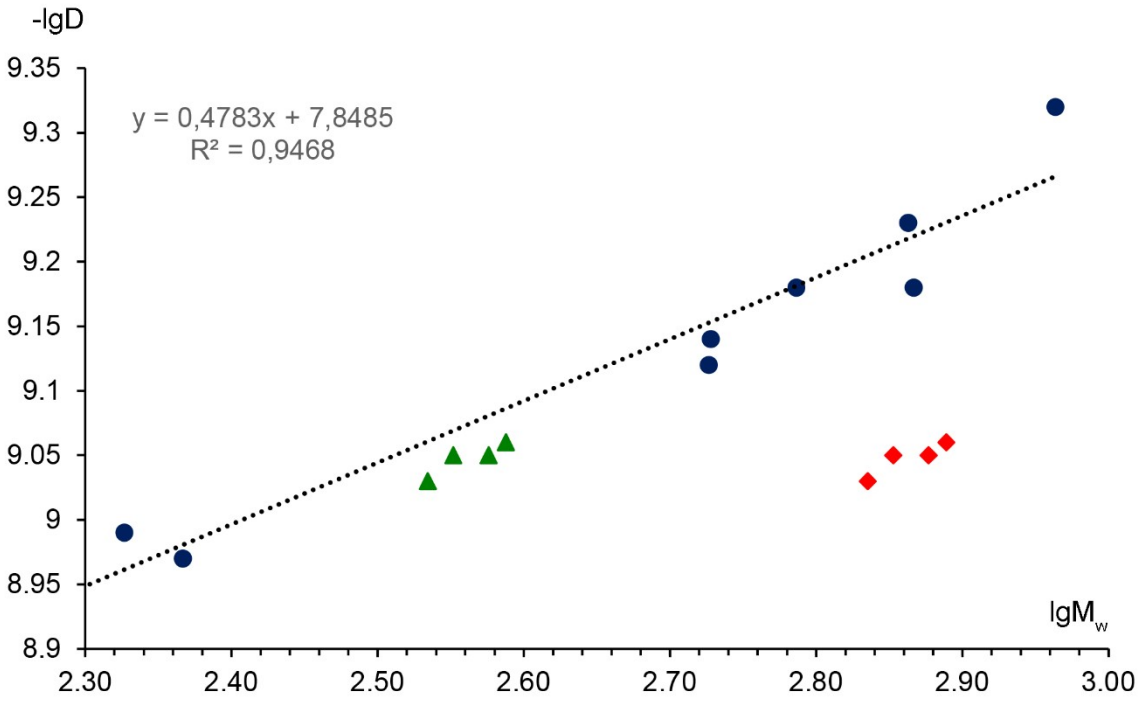


Fig. S15. Dependence of log *D vs* log M_w in $CDCl_3$ (where D – diffusion coefficient, M_w - molecular weight). All compounds were normalized to log $D_{ref,fix}$(Naphthalene) = −8.79 [7]. Blue circles calculated for previously published compounds, green triangles – for monomeric species of **1-4**, red squares – for dimeric species of **1-4**. For data see Table S3.

1. Milani, N.C., et al., *A new class of copper(I) complexes with imine-containing chelators which show potent anticancer activity.* Appl. Organomet. Chem., 2020. **34**(4): p. e5526.
2. Qiao, X., et al., *Study on potential antitumor mechanism of a novel Schiff Base copper(II) complex: Synthesis, crystal structure, DNA binding, cytotoxicity and apoptosis induction activity.* J. Inorg. Biochem., 2011. **105**(5): p. 728-737.
3. Piskunov, A.V., et al., *Template Synthesis of Tin(IV) Complexes with Tridentate Iminopyridine Ligands.* Russ. J. Coord. Chem., 2019. **45**(3): p. 188-199.
4. Piskunov, A.V., et al., *Template Assembling of the Pentadentate Redox-Active Ligand in the Coordination Sphere of Tin(IV).* Russ. J. Coord. Chem., 2018. **44**(2): p. 138-146.
5. Piskunov, A.V., et al., *Tin(iv) and lead(iv) complexes with a tetradentate redox-active ligand.* Dalton Trans., 2012. **41**(36): p. 10970-10979.
6. Cherkasov, V.K., et al., *A New Octacoordinated Tin Complex with Tetradentate RedoxActive Ligands.* Doklady Chemistry, 2013. **448**: p. 61-65.
7. Neufeld, R. and D. Stalke, *Accurate molecular weight determination of small molecules via DOSY-NMR by using external calibration curves with normalized diffusion coefficients.* Chem. Sci., 2015. **6**: p. 3354-3364.

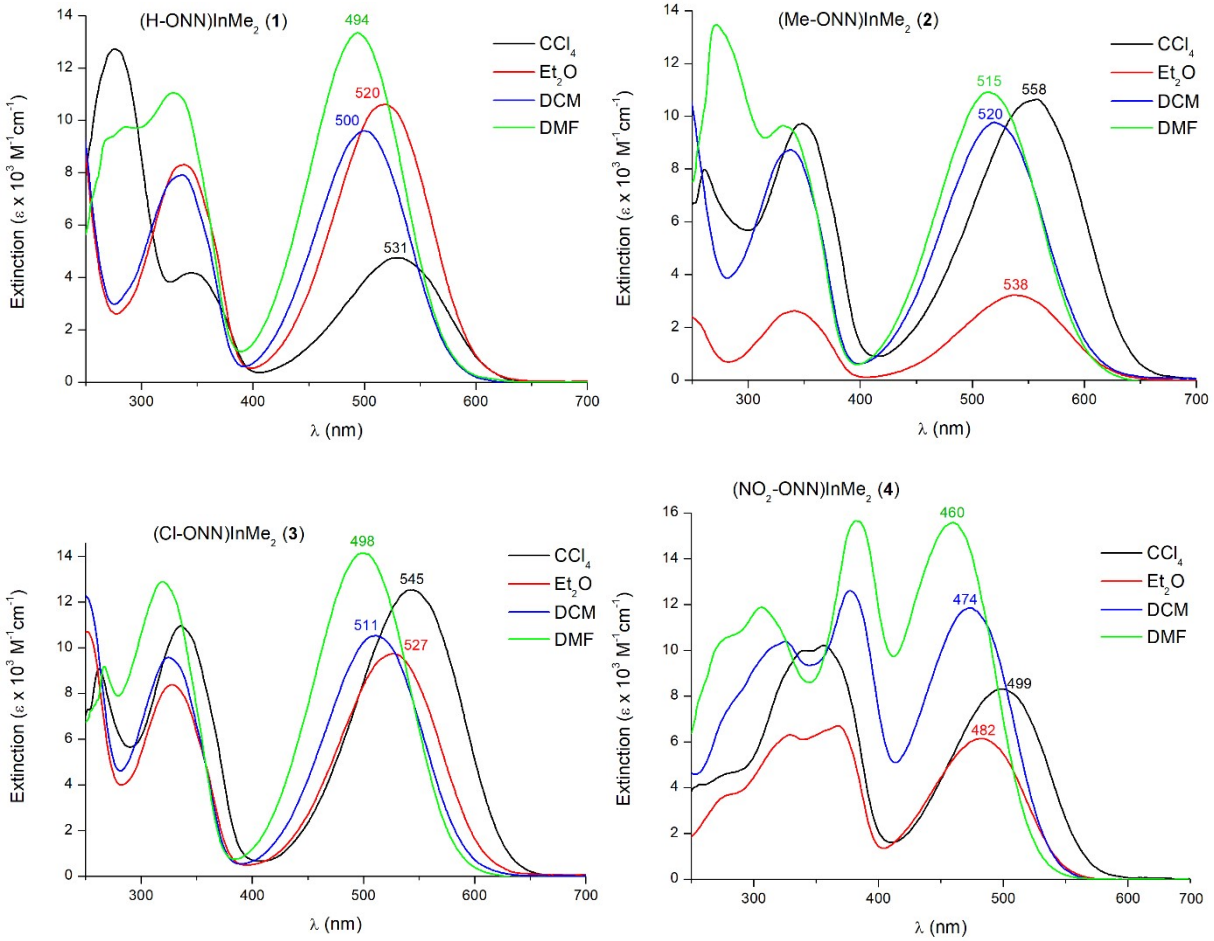


Fig. S16. UV-vis absorption spectra of **1-4** in various organic solvents at 293 K (C = 10^{-4} M).

Table S4. Electronic absorption spectral data of **1-4** in CCl_4, Et_2O, DCM, DMF at 293 K.

Complex	Solvent	λ_{max}, nm (ε x 10^{-4} M^{-1} cm^{-1})				
1	CCl_4	276 (1.27),	345 (0.42),	531 (0.47)		
	Et_2O	238 (1.17),	339 (0.83),	520 (1.06)		
	DCM	239 (1.17),	336 (0.79),	500 (0.96)		
	DMF	274sh (0.94),	286sh (0.98),	330 (1.10),	494 (1.33)	
2	CCl_4	261 (0.80),	348 (0.97),	558 (1.06)		
	Et_2O	233 (0.30),	259sh (0.20),	341 (0.26),	538 (0.32)	
	DCM	235 (1.26),	337 (0.87),	520 (0.98)		
	DMF	272 (1.35),	331 (0.96),	515 (1.09)		
3	CCl_4	262 (0.91),	336 (1.10),	545 (1.25)		
	Et_2O	232 (1.19),	251sh (1.07),	328 (0.84),	527 (0.97)	
	DCM	237 (1.25),	251sh (1.22),	324 (0.96),	511 (1.05)	
	DMF	267 (0.92),	320 (1.29),	498 (1.41)		
4	CCl_4	341sh (1.00),	356 (1.02),	499 (0.83)		
	Et_2O	224 (0.50),	276sh (0.36),	329 (0.63),	368 (0.67),	482 (0.61)
	DCM	230 (0.76),	325 (1.04),	377 (1.26),	474 (1.18)	
	DMF	277sh (1.05),	306 (1.19),	382 (1.57),	460 (1.56)	

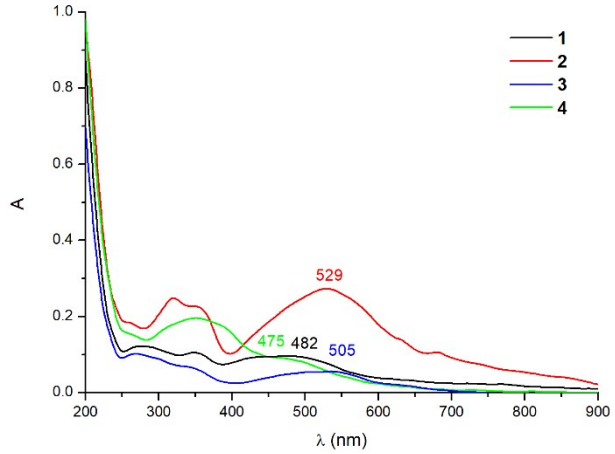


Fig. S17. UV-vis absorption spectra of **1-4** recorded in Nujol at 293 K.

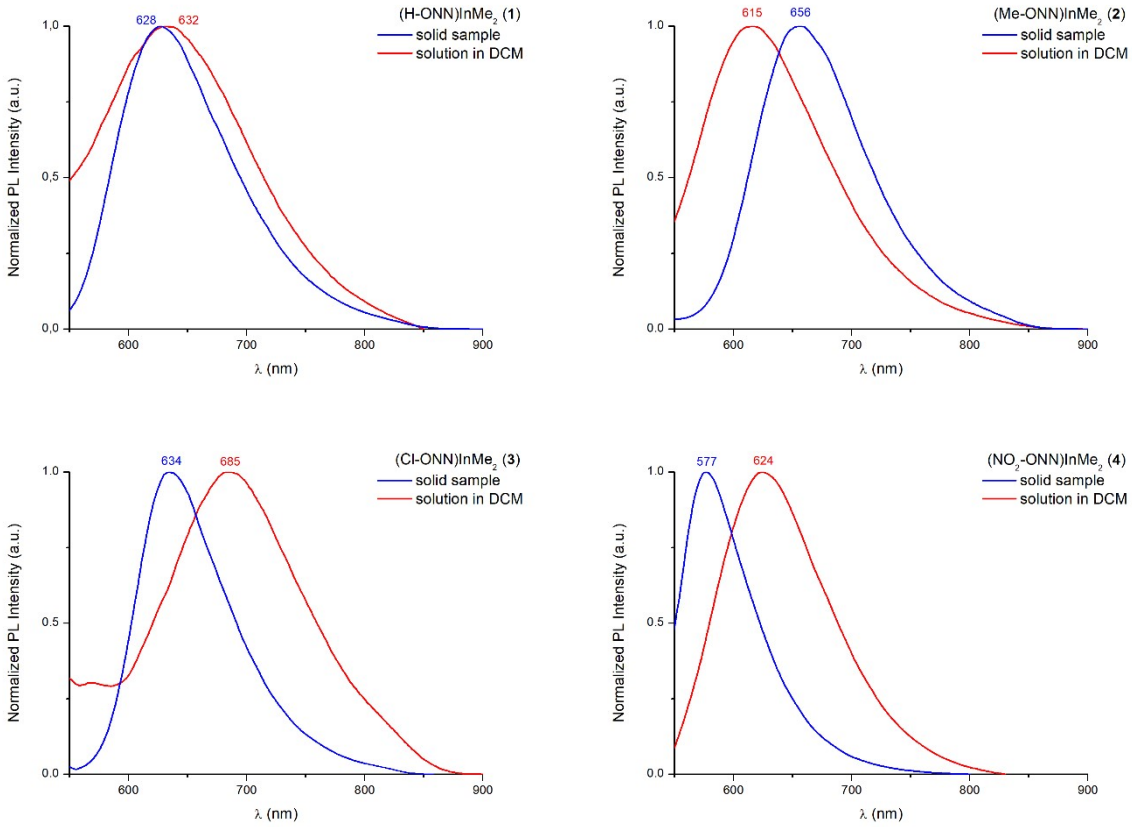


Fig. S18. PL spectra of **1-4** recorded in solid state and in DCM solution (C = 10^{-5} M) at 293 K.

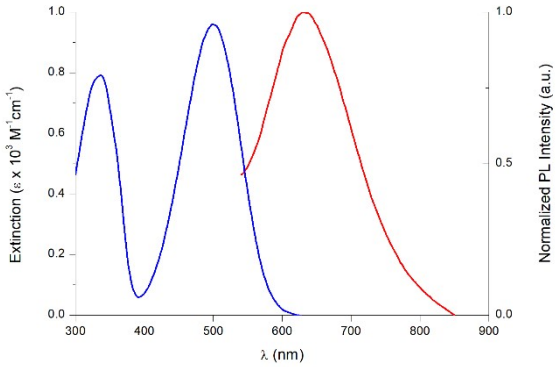


Fig. S19. UV-PL spectra of **1** in DCM at 293 K.

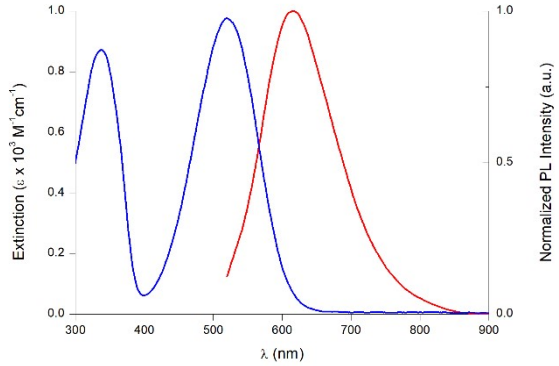


Fig. S20. UV-PL spectra of **2** in DCM at 293 K.

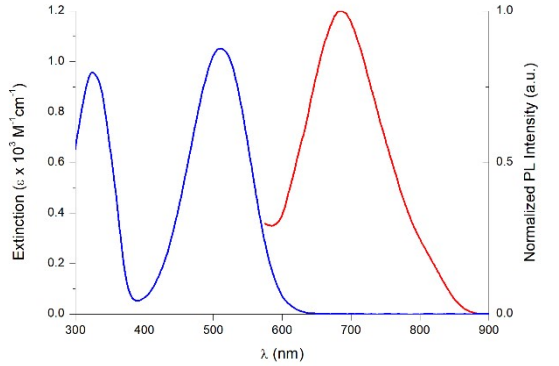


Fig. S21. UV-PL spectra of **3** in DCM at 293 K.

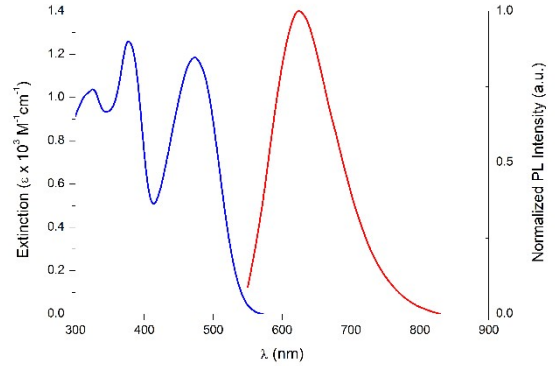


Fig. S22. UV-PL spectra of **4** in DCM at 293 K.

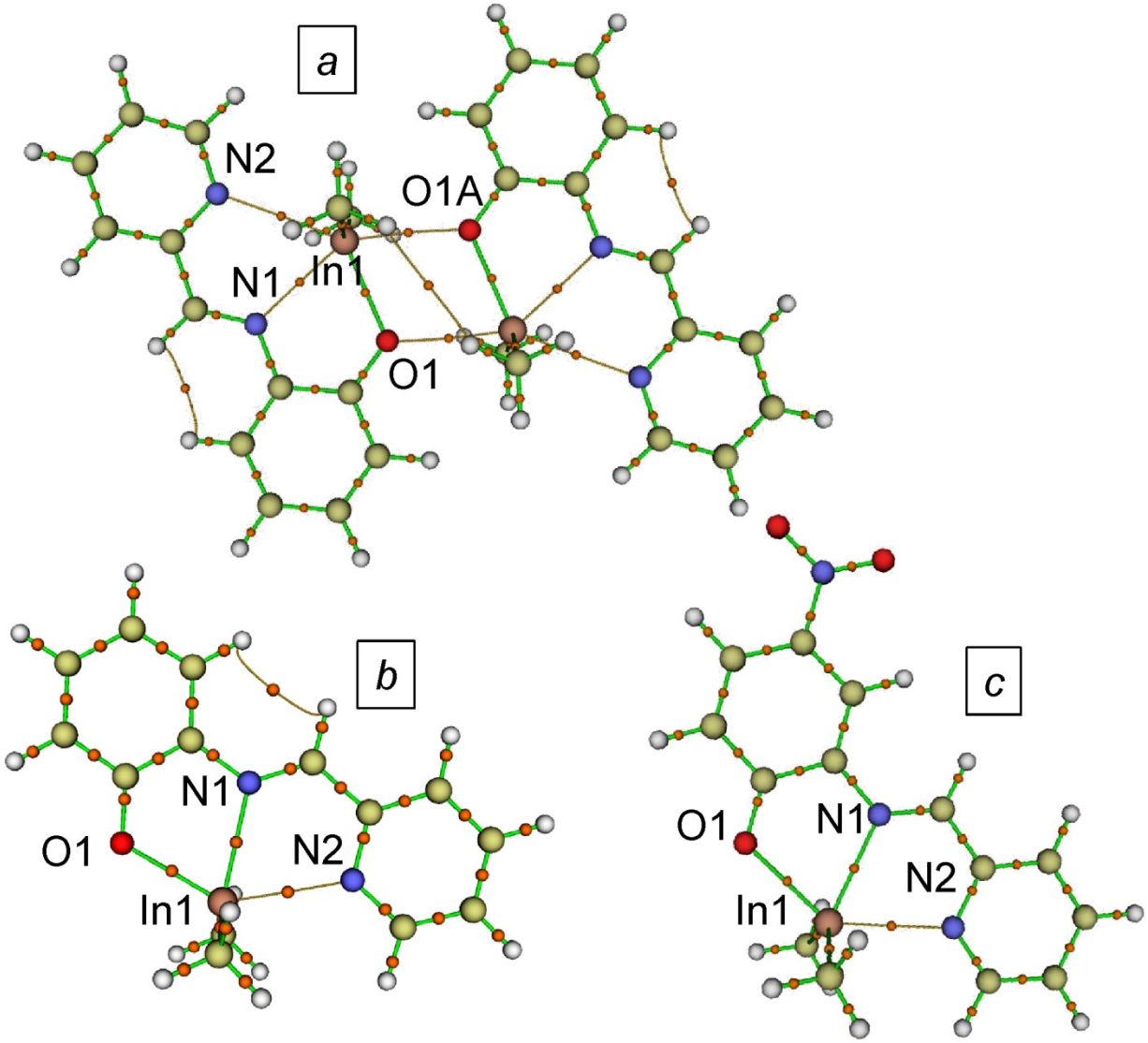


Fig. S23. Molecular graphs of the DFT-optimized **1** dimer (a) and monomers **1** (b) and **4** (c). The small orange circles correspond to the (3,-1) bonding critical points.

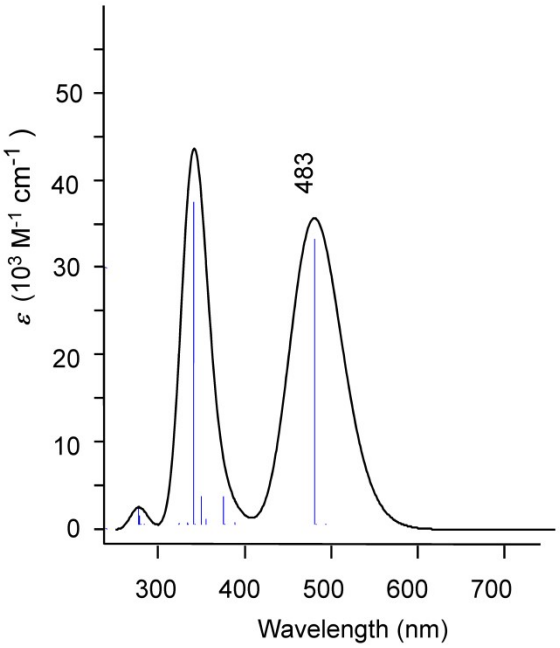


Fig. S24. Calculated absorption spectrum of the **1** dimer. The long-wavelength peak maximum (nm) is indicated.

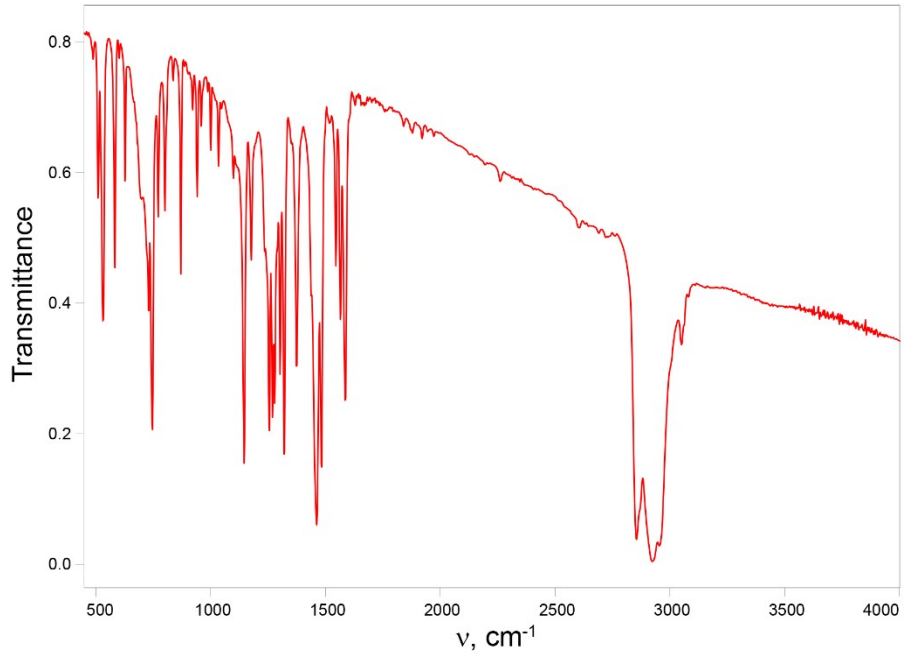


Fig. S25. IR spectrum of **1**.

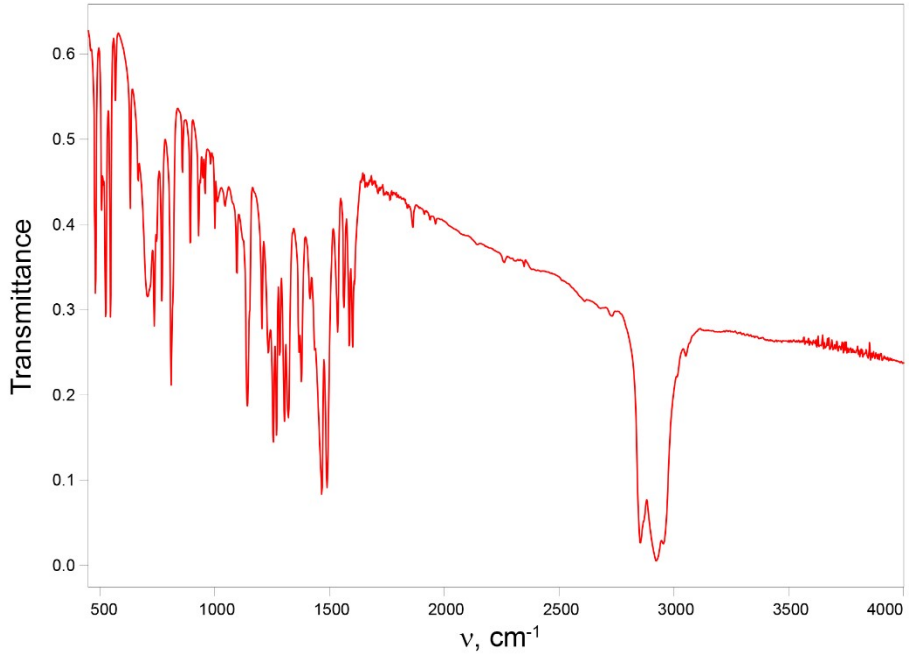


Fig. S26. IR spectrum of **2**.

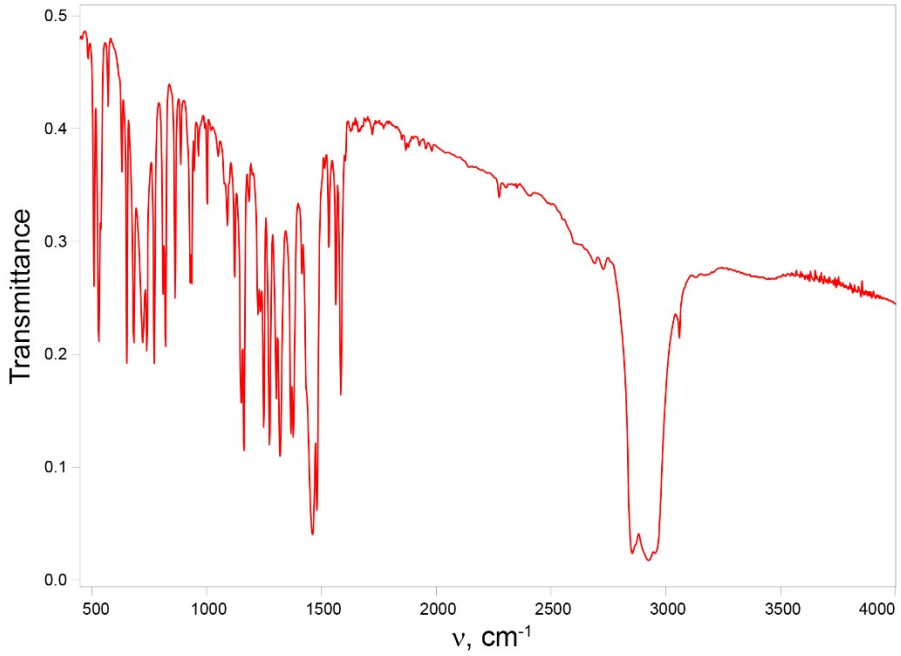


Fig. S27. IR spectrum of **3**.

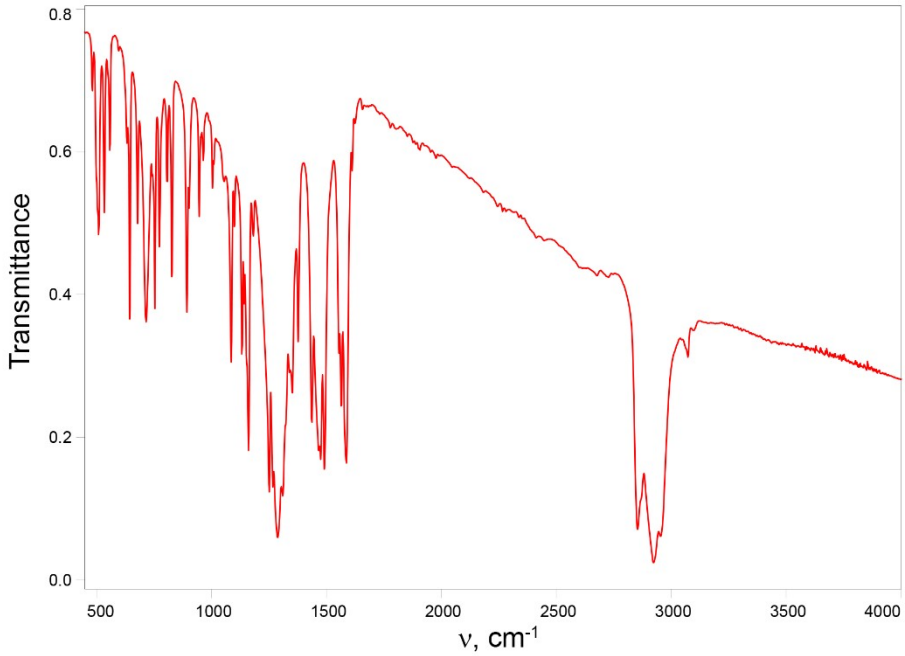


Fig. S28. IR spectrum of **4**.

Atomic coordinates in the optimized structures of dimer **1** and **1**, **4** monomers.

66

1 dimer, S0, E = -1835.54984445 a.u.

In	1.921100	0.562900	-0.000200
O	0.657400	-1.278700	0.000500
N	3.375500	-1.437500	0.000000
N	4.690200	1.030700	-0.000200
C	2.006000	1.156800	2.079400
H	2.723900	0.532500	2.609300
H	1.020800	1.033300	2.523700
H	2.309700	2.198400	2.178300
C	2.006000	1.156100	-2.079900
H	1.020900	1.032300	-2.524400
H	2.724100	0.531900	-2.609700
H	2.309300	2.197700	-2.178900
C	1.214000	-2.451500	0.000200
C	0.429000	-3.633400	0.000200
H	-0.646600	-3.525900	0.000300
C	1.006600	-4.881200	-0.000000
H	0.374900	-5.760800	-0.000100
C	2.402700	-5.029900	-0.000300
H	2.848800	-6.014700	-0.000500
C	3.196700	-3.905800	-0.000200
H	4.271600	-4.027400	-0.000500
C	2.638100	-2.614700	0.000000
C	4.657700	-1.378700	0.000300
H	5.275700	-2.275400	0.000600
C	5.388500	-0.116000	0.000200
C	6.788800	-0.122400	0.000400
H	7.323700	-1.062700	0.000700
C	7.469700	1.083900	0.000300
H	8.551500	1.102500	0.000500
C	6.740400	2.265900	-0.000100
H	7.228000	3.230400	-0.000200
C	5.351100	2.180900	-0.000300
H	4.746100	3.080700	-0.000600
In	-1.921100	-0.562900	0.000200
O	-0.657400	1.278700	-0.000500
N	-3.375500	1.437500	-0.000000
N	-4.690200	-1.030700	0.000200
C	-2.006000	-1.156800	-2.079400
H	-2.723900	-0.532500	-2.609300
H	-1.020900	-1.033300	-2.523700
H	-2.309700	-2.198400	-2.178300
C	-2.006000	-1.156100	2.079900
H	-1.020900	-1.032300	2.524400
H	-2.724100	-0.531900	2.609700
H	-2.309300	-2.197700	2.178900

C -1.214000 2.451500 -0.000200
C -0.429000 3.633400 -0.000200
H 0.646600 3.525900 -0.000300
C -1.006600 4.881200 0.000100
H -0.374900 5.760800 0.000100
C -2.402700 5.029900 0.000300
H -2.848800 6.014700 0.000500
C -3.196800 3.905800 0.000300
H -4.271600 4.027400 0.000500
C -2.638100 2.614800 -0.000000
C -4.657700 1.378700 -0.000300
H -5.275700 2.275400 -0.000600
C -5.388500 0.116000 -0.000100
C -6.788800 0.122300 -0.000400
H -7.323700 1.062700 -0.000700
C -7.469700 -1.083900 -0.000300
H -8.551500 -1.102500 -0.000500
C -6.740400 -2.265900 0.000100
H -7.227900 -3.230400 0.000200
C -5.351100 -2.180900 0.000300
H -4.746100 -3.080700 0.000500
66
1 dimer (+D3), S0, E = -1835.62638846 a.u.
In -1.866300 0.561600 0.000200
O -0.602600 -1.278200 0.000700
N -3.311300 -1.467500 -0.000100
N -4.609500 0.995000 -0.000800
C -1.963200 1.122000 -2.083000
H -2.717000 0.522400 -2.591700
H -0.989500 0.946000 -2.536600
H -2.218700 2.175400 -2.196400
C -1.964400 1.122200 2.083200
H -0.991000 0.946200 2.537300
H -2.718500 0.522700 2.591500
H -2.219800 2.175600 2.196500
C -1.142900 -2.459300 0.001000
C -0.342000 -3.628600 0.001900
H 0.731900 -3.506800 0.002300
C -0.904600 -4.883900 0.002200
H -0.262200 -5.755700 0.002800
C -2.298600 -5.049500 0.001700
H -2.732200 -6.039800 0.002000
C -3.107400 -3.935300 0.000900
H -4.180800 -4.069100 0.000700
C -2.564400 -2.638000 0.000600
C -4.593000 -1.412300 -0.000900
H -5.212700 -2.308400 -0.001200
C -5.318000 -0.145500 -0.001300

C -6.718100 -0.138200 -0.002300
H -7.263300 -1.072600 -0.002700
C -7.386300 1.075900 -0.002700
H -8.467700 1.105600 -0.003400
C -6.645400 2.251100 -0.002100
H -7.123800 3.220200 -0.002400
C -5.256600 2.152100 -0.001200
H -4.639100 3.043300 -0.000700
In 1.866300 -0.561600 0.000200
O 0.602600 1.278200 0.000800
N 3.311300 1.467500 0.000000
N 4.609500 -0.995000 -0.000900
C 1.964300 -1.122300 2.083200
H 2.718400 -0.522800 2.591600
H 0.990900 -0.946300 2.537300
H 2.219800 -2.175700 2.196400
C 1.963200 -1.121900 -2.083000
H 0.989600 -0.946000 -2.536600
H 2.717000 -0.522300 -2.591600
H 2.218800 -2.175300 -2.196500
C 1.142900 2.459300 0.001200
C 0.342000 3.628600 0.002100
H -0.731900 3.506800 0.002500
C 0.904600 4.883900 0.002500
H 0.262200 5.755700 0.003200
C 2.298600 5.049500 0.002000
H 2.732100 6.039900 0.002400
C 3.107400 3.935300 0.001200
H 4.180800 4.069100 0.001000
C 2.564400 2.638000 0.000800
C 4.593000 1.412300 -0.000700
H 5.212800 2.308400 -0.001000
C 5.318000 0.145500 -0.001300
C 6.718100 0.138200 -0.002200
H 7.263300 1.072600 -0.002500
C 7.386300 -1.075900 -0.002700
H 8.467700 -1.105600 -0.003400
C 6.645400 -2.251100 -0.002300
H 7.123800 -3.220200 -0.002600
C 5.256500 -2.152100 -0.001400
H 4.639100 -3.043300 -0.001000
33
1 monomer, S0, E = -917.784427637 a.u.
In 0.211100 -1.371700 -0.000300
O -2.031400 -1.357900 0.001100
N -0.497400 0.877700 0.000200
N 2.167600 0.244700 0.000200
C 0.590600 -2.077300 -2.021900

H 0.369200 -1.281300 -2.732300
H -0.046800 -2.932800 -2.242300
H 1.632600 -2.373100 -2.137000
C 0.592500 -2.080400 2.019900
H -0.045100 -2.935800 2.239700
H 0.372400 -1.285300 2.731700
H 1.634500 -2.377000 2.133300
C -2.618600 -0.205300 0.000700
C -4.035700 -0.101500 0.000800
H -4.606100 -1.021200 0.001100
C -4.665500 1.122500 0.000300
H -5.747600 1.165000 0.000400
C -3.925800 2.318400 -0.000200
H -4.431500 3.273900 -0.000700
C -2.548900 2.260200 -0.000300
H -1.982900 3.182000 -0.000800
C -1.877600 1.025200 0.000200
C 0.367500 1.827900 0.000400
H 0.082500 2.876400 0.000700
C 1.796000 1.537300 0.000300
C 2.737100 2.569200 0.000400
H 2.407600 3.598900 0.000600
C 4.086200 2.248600 0.000300
H 4.833500 3.030000 0.000300
C 4.461300 0.911000 0.000100
H 5.500500 0.616500 0.000000
C 3.462200 -0.056800 0.000100
H 3.713100 -1.110300 -0.000100
33
1 monomer, S1, E = -917.774368084 a.u.
In -0.294800 -1.340500 0.033000
O 2.073800 -1.319800 -0.374000
N 0.503100 0.798700 0.029400
N -2.151400 0.249200 0.156900
C -0.268600 -2.158000 2.048900
H 0.013500 -1.379400 2.756800
H 0.449900 -2.974100 2.114700
H -1.255300 -2.536300 2.315400
C -0.790800 -2.114500 -1.938900
H -0.119200 -2.931200 -2.201300
H -0.685200 -1.319600 -2.676900
H -1.817400 -2.479400 -1.958800
C 2.672800 -0.196200 -0.233300
C 4.086200 -0.076800 -0.285000
H 4.657200 -0.964900 -0.519900
C 4.712000 1.138800 -0.029700
H 5.790200 1.212000 -0.071100
C 3.949800 2.258000 0.272600

H 4.426900 3.209300 0.462600
C 2.535800 2.175700 0.319600
H 1.968900 3.056900 0.588000
C 1.891800 0.999000 0.025000
C -0.350800 1.779200 -0.160500
H -0.014100 2.784200 -0.398700
C -1.752500 1.538100 -0.084700
C -2.698400 2.570200 -0.243400
H -2.355500 3.576600 -0.443400
C -4.041500 2.285300 -0.132600
H -4.778900 3.067700 -0.247200
C -4.437600 0.963400 0.130600
H -5.479300 0.694500 0.225400
C -3.454700 -0.007400 0.258000
H -3.727000 -1.039500 0.445200
33
1 monomer, T1, E = -917.733096653 a.u.
In -0.289400 -1.327200 0.000000
O 2.113200 -1.361900 -0.000000
N 0.525500 0.794500 0.000000
N -2.149100 0.232100 0.000000
C -0.519000 -2.136800 2.007300
H -0.276600 -1.368400 2.740800
H 0.148300 -2.985700 2.151400
H -1.545600 -2.465200 2.168000
C -0.519000 -2.136800 -2.007300
H 0.148400 -2.985600 -2.151400
H -0.276700 -1.368400 -2.740800
H -1.545600 -2.465300 -2.168000
C 2.683700 -0.229600 -0.000000
C 4.104400 -0.103200 -0.000000
H 4.683600 -1.016700 -0.000000
C 4.701600 1.130300 -0.000000
H 5.779300 1.218100 -0.000000
C 3.906200 2.299300 0.000000
H 4.391100 3.266600 0.000000
C 2.525100 2.240500 0.000000
H 1.962700 3.162100 0.000000
C 1.859100 0.999400 0.000000
C -0.374400 1.816400 -0.000000
H -0.052900 2.849000 -0.000000
C -1.754600 1.544800 -0.000000
C -2.723900 2.580200 -0.000000
H -2.394500 3.610400 -0.000000
C -4.060200 2.261400 -0.000000
H -4.807900 3.042800 -0.000000
C -4.444500 0.911400 0.000000
H -5.484000 0.619200 0.000000

C -3.448100 -0.054900 0.000000
H -3.706400 -1.107400 0.000000
35
4 monomer, S0, E = -1122.38542224 a.u.
In -1.423600 -1.396600 0.000000
O 0.697900 -2.232400 -0.000100
N 0.109900 0.407600 -0.000000
N -2.592400 0.844400 0.000000
C -1.989700 -1.897800 2.032700
H -1.489700 -1.221300 2.724800
H -1.691800 -2.920500 2.259200
H -3.067000 -1.804300 2.161700
C -1.990100 -1.898000 -2.032500
H -1.692000 -2.920600 -2.259000
H -1.490200 -1.221500 -2.724700
H -3.067400 -1.804600 -2.161300
C 1.670900 -1.404900 -0.000100
C 3.026500 -1.852200 -0.000100
H 3.201300 -2.919200 -0.000100
C 4.073900 -0.972600 -0.000100
H 5.094200 -1.324200 -0.000100
C 3.822300 0.411600 -0.000000
C 2.524600 0.902100 -0.000000
H 2.381100 1.971300 0.000000
C 1.450800 0.023800 -0.000100
C -0.322000 1.613700 -0.000100
H 0.342900 2.473400 -0.000100
C -1.754400 1.895800 -0.000100
C -2.220800 3.209600 -0.000100
H -1.518800 4.031600 -0.000100
C -3.590500 3.434600 -0.000000
H -3.978800 4.443400 -0.000100
C -4.449900 2.345100 0.000000
H -5.522400 2.473400 0.000000
C -3.902500 1.065000 0.000000
H -4.541300 0.190800 0.000100
N 4.923100 1.336900 0.000000
O 4.683700 2.547100 0.000100
O 6.070900 0.886700 0.000000
35
4 monomer, S1, E = -1122.37793022 a.u.
In -1.527400 -1.291400 0.000100
O 0.736800 -2.238100 -0.001700
N 0.071800 0.350800 -0.000300
N -2.608400 0.860700 0.000700
C -1.987200 -1.948600 2.018600
H -1.456000 -1.321300 2.733500
H -1.680400 -2.984200 2.157200

H -3.057700 -1.868700 2.204600
C -1.989900 -1.947800 -2.017900
H -1.683300 -2.983300 -2.157400
H -1.459700 -1.320300 -2.733300
H -3.060700 -1.867800 -2.202500
C 1.695200 -1.417500 -0.001200
C 3.056600 -1.856900 -0.001400
H 3.237700 -2.922100 -0.002400
C 4.095400 -0.955500 -0.000200
H 5.123500 -1.280800 -0.000400
C 3.801200 0.407300 0.001100
C 2.479500 0.903000 0.001200
H 2.339800 1.971000 0.002500
C 1.419900 0.022700 -0.000100
C -0.343700 1.608400 -0.001400
H 0.351700 2.439900 -0.002900
C -1.729800 1.910900 -0.000900
C -2.198500 3.242100 -0.001900
H -1.483900 4.053900 -0.003200
C -3.553900 3.486100 -0.001300
H -3.927100 4.500800 -0.002000
C -4.441500 2.400300 0.000400
H -5.511600 2.545400 0.001000
C -3.914800 1.115400 0.001300
H -4.572600 0.254500 0.002500
N 4.893600 1.357800 0.002200
O 4.614400 2.558400 0.003100
O 6.049500 0.932200 0.002300
35
4 monomer, T1, E = -1122.32561489 a.u.
In -1.501600 -1.304600 0.000100
O 0.732400 -2.262800 0.000600
N 0.095200 0.336000 0.000200
N -2.585900 0.864200 -0.000200
C -1.984000 -1.943000 2.019100
H -1.429300 -1.336300 2.733700
H -1.716100 -2.989300 2.157200
H -3.050600 -1.823000 2.205200
C -1.983000 -1.943500 -2.018800
H -1.715500 -2.990000 -2.156400
H -1.427600 -1.337400 -2.733400
H -3.049400 -1.823100 -2.205700
C 1.683100 -1.443800 0.000400
C 3.051000 -1.866700 0.000400
H 3.243400 -2.930100 0.000700
C 4.070100 -0.962300 0.000000
H 5.101600 -1.276400 0.000000
C 3.769300 0.421600 -0.000400

C	2.481700	0.915300	-0.000400
H	2.334600	1.981600	-0.000700
C	1.392100	0.015700	0.000000
C	-0.337300	1.637800	0.000300
H	0.362400	2.461400	0.000600
C	-1.712800	1.920200	0.000100
C	-2.200300	3.251800	0.000300
H	-1.494800	4.071000	0.000600
C	-3.556300	3.478700	0.000200
H	-3.941000	4.489300	0.000300
C	-4.433000	2.386100	-0.000200
H	-5.504300	2.520700	-0.000300
C	-3.892000	1.105000	-0.000400
H	-4.541000	0.237500	-0.000600
N	4.876200	1.366400	-0.000700
O	4.618600	2.568100	-0.001000
O	6.022900	0.921000	-0.000800