Electronic Supplementary Information

Bio-based 1,3-diisobutyl imidazolium hydrogen oxalate [iBu2IM](HC2O4) as CO2 shuttle

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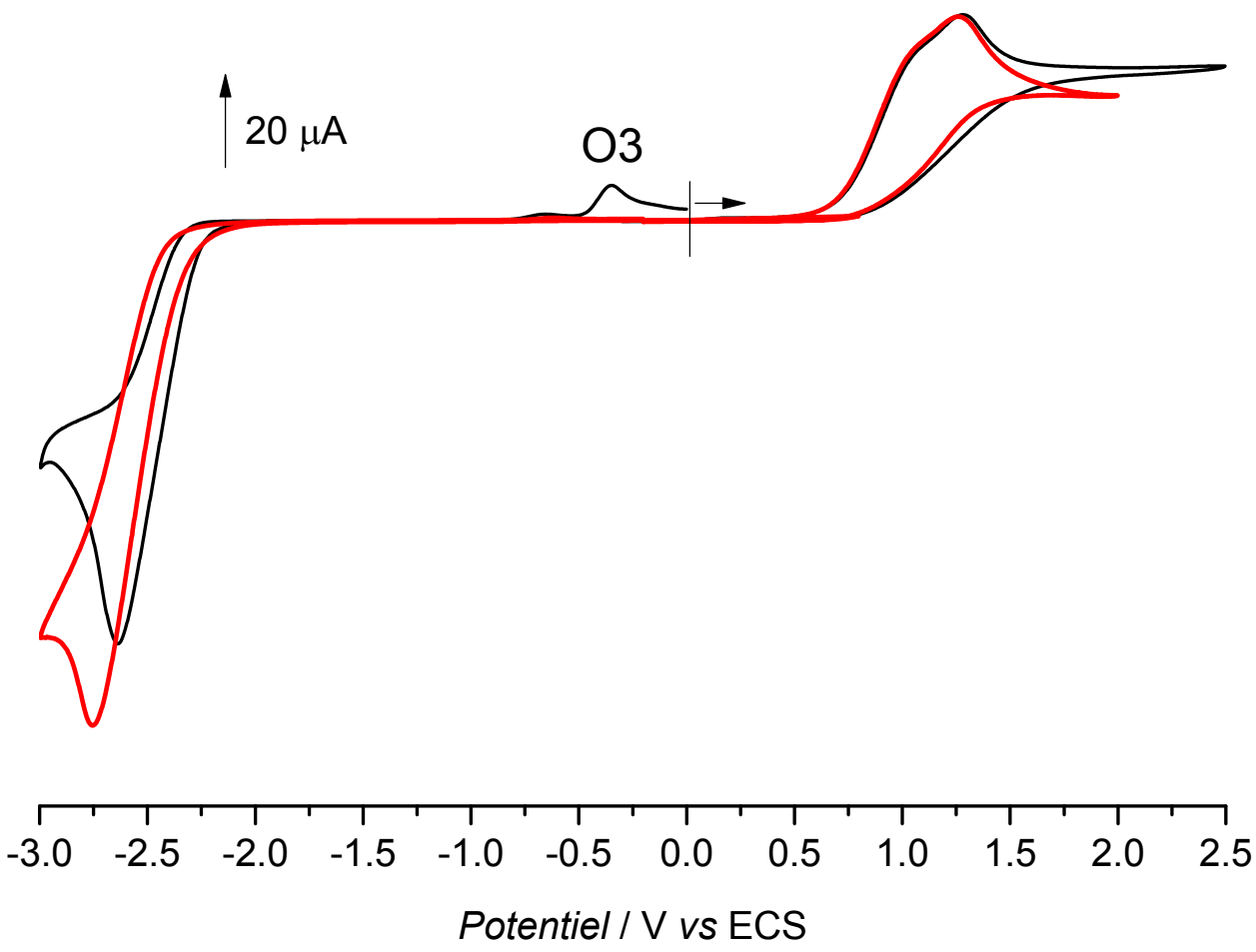
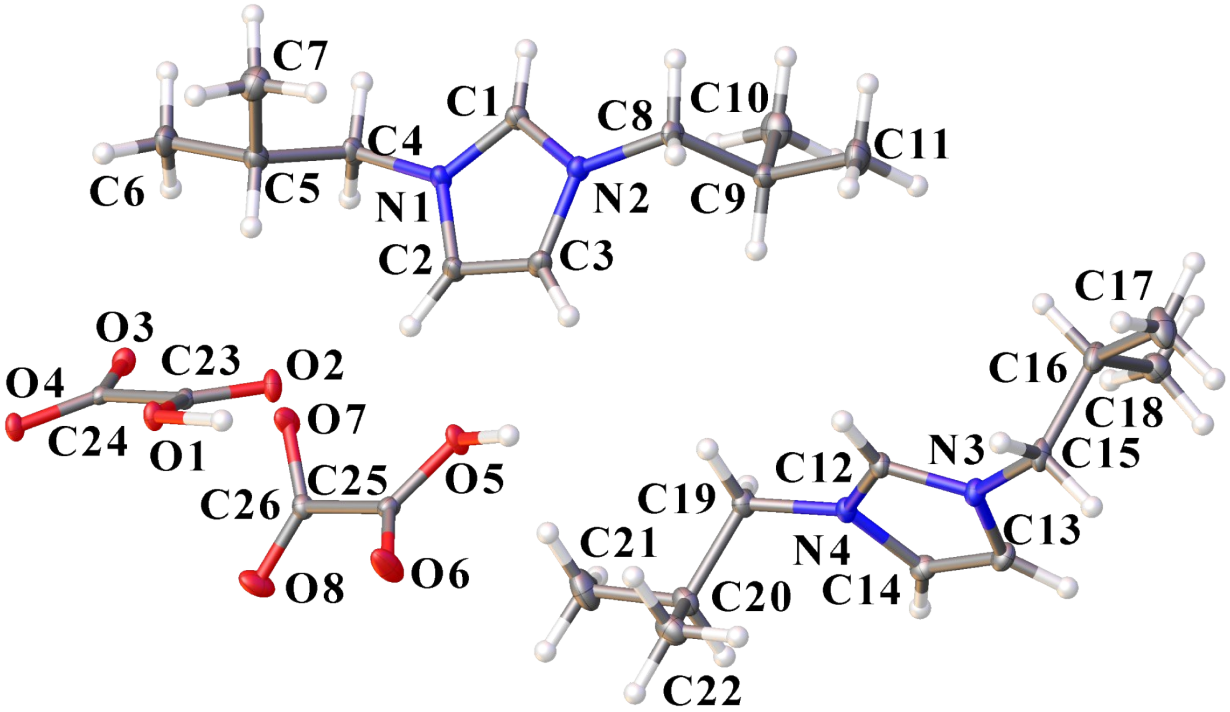
Cyclic voltammograms of [*i*Bu$_2$IM](HC$_2$O$_4$). They were performed at RT with v = 100 mV s^{-1} under argon (black line) and under CO_2 bubbling (red line) in CH_3CN 0.1 M $TBAPF_6$ with C = 3.1x10^{-2} M (working electrode: glassy carbon Ø = 3 mm, reference electrode: SCE and CE: Pt)



X-ray structure analyses

X-Ray analysis of [*i*Bu$_2$IM](HC$_2$O$_4$) and [*i*Bu$_2$IM](HCO$_3$) compounds. Single crystals of [*i*Bu$_2$IM](HC$_2$O$_4$) were obtained from ethanol/THF mixture. A suitable crystal of [*i*Bu$_2$IM](HC$_2$O$_4$) was selected and mounted on a mylar loop with grease on a Bruker D8 VENTURE diffractometer. The crystal was kept at 100 K during data collection. A suitable crystal of [*i*Bu$_2$IM](HCO$_3$) was selected and mounted on a glass fibre with superglue on a Bruker APEX-II CCD diffractometer. The crystal was kept at 298 K during data collection. Data were measured using ϕ and ω scans using MoK$_\alpha$ radiation (X-ray tube). The total number of runs and images was based on the strategy calculation from the program APEX2 (Bruker, 2014).[1] The structures were solved by intrinsic phasing methods (ShelXT, 2008)4 and refined with full-matrix least-squares methods based on F2 (ShelXL)[2] with the aid of the Olex2 program.[3] All non-hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atoms attached to carbon atoms were included in calculated positions and refined as riding atoms. Crystal data of [*i*Bu$_2$IM](HC$_2$O$_4$) and [*i*Bu$_2$IM](HCO$_3$) compounds were deposited at the CCDC under the 1560697 and 1560698 reference numbers.

Crystal structure of [*i*Bu$_2$IM](HC$_2$O$_4$) – view 1 with labelled atoms



Crystal structure of [*i*Bu_2IM](HC_2O_4) – view 2

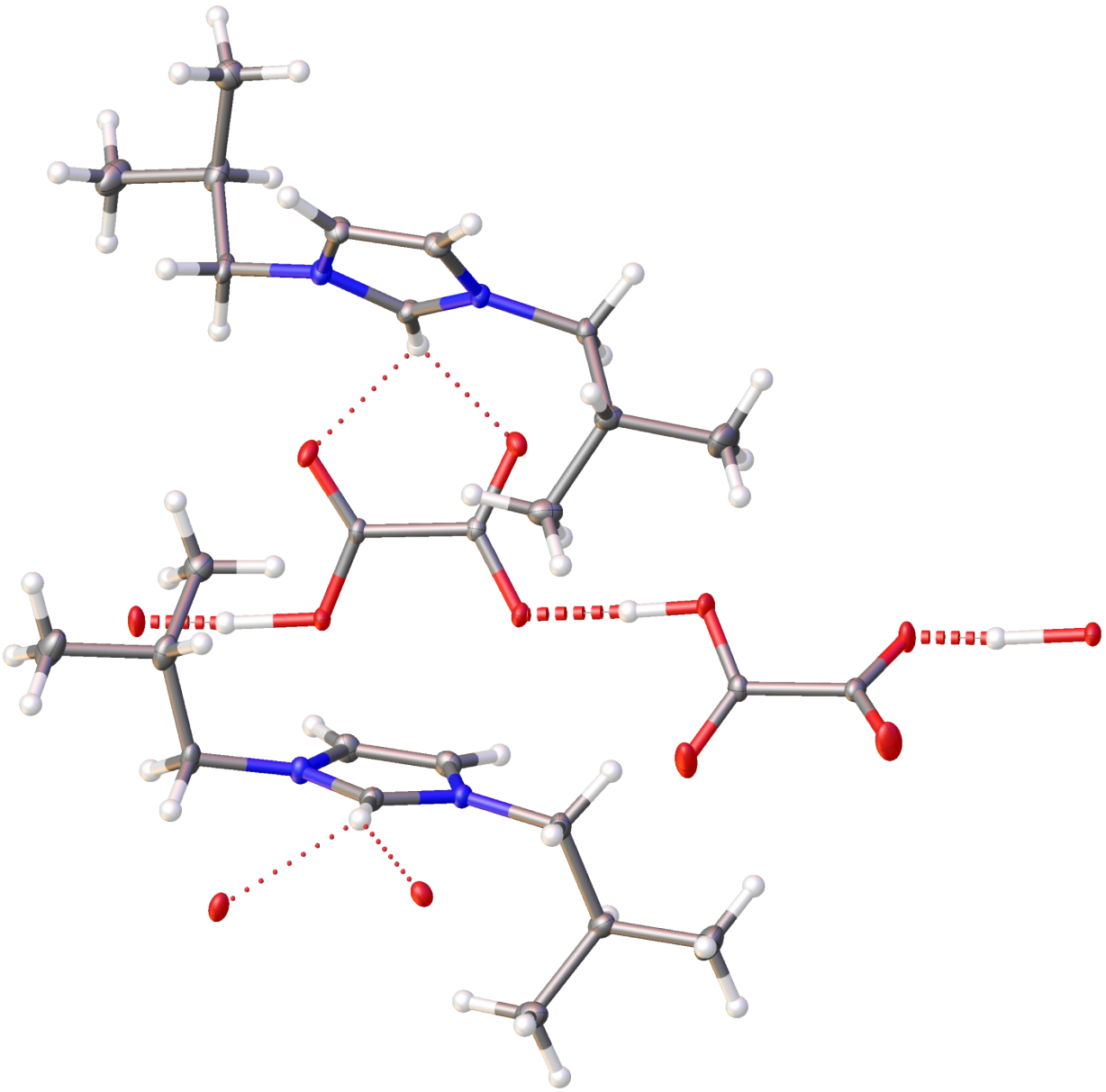


Table 1. Crystal data and structure refinement for [*i*Bu_2IM](HC_2O_4)

CCDC	1560697
Formula	$C_{26}H_{44}N_4O_8$
$D_{calc.}$ / g cm^{-3}	1.182
μ / mm^{-1}	0.088
Formula Weight	540.65
Colour	colourless
Shape	prism
Size / mm^3	0.40 × 0.35 × 0.10
T / K	100
Crystal System	orthorhombic
Space Group	*Pca2$_1$*
a / Å	22.5633(11)
b / Å	10.2111(5)
c / Å	13.1867(5)
α / °	90
β / °	90
γ / °	90
V = Å^3	3038.2(2)
Z	4
Θ_{min} / °	3.090
Θ_{max} / °	27.517
Measured Refl.	55853
Independent Refl.	6599
Reflections Used	5365
R_{int}	0.0552
Parameters	358
Restraints	1
Largest Peak Largest Peak	0.268
Deepest Hole	-0.168
GooF	1.014
ωR_2 (all data)	0.0805
ωR_2	0.0744
R_1 (all data)	0.0581
R_1	0.0379

Table 2. Fractional Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^{2}x10^3) for [*i*Bu_2IM](HC_2O_4). *U(eq)* is defined as one third of the trace of the orthogonalized *Uij* tensor.

Atom	x	y	z	U_{eq}
C12	7151.1(10)	7399(2)	3655.1(18)	18.9(5)
C13	8000.5(10)	8049(2)	3003.2(18)	22.8(5)
C14	8033(1)	6743(2)	3135.8(17)	21.4(5)
C15	7208.0(11)	9784(2)	3271.7(19)	24.1(5)
C16	6884.9(11)	10047(2)	2275(2)	28.4(6)
C17	6671.1(13)	11463(3)	2295(2)	41.9(7)
C18	7272.1(12)	9791(2)	1349(2)	31.0(6)
C19	7348.7(10)	5009(2)	3854.0(18)	21.4(5)
C20	7705.3(10)	4555(2)	4772.9(18)	23.9(5)
C21	7564.5(15)	3105(2)	4950(2)	43.3(7)
C22	7576.9(12)	5382(3)	5705.8(19)	31.6(6)
N3	7447.0(8)	8441.8(17)	3328.3(14)	19.7(4)
N4	7496.8(8)	6349.7(16)	3545.0(14)	18.0(4)
C1	4972.4(10)	2644.5(19)	3091.3(18)	18.7(5)
C2	5574.9(10)	2217(2)	4367.0(17)	22.3(5)
C3	5599.9(11)	3515(2)	4181.0(17)	22.9(5)
C4	5015.9(10)	293(2)	3651.4(19)	22.7(5)
C5	4719.0(11)	-113(2)	4645.4(19)	26.6(5)
C6	4613.4(12)	-1599(2)	4634(2)	33.6(6)
C7	4147.9(12)	629(3)	4831(2)	37.5(6)
C8	5131.5(10)	5075(2)	2943.7(18)	22.2(5)
C9	5646.4(10)	5488(2)	2269.6(19)	23.6(5)
C10	5666.4(13)	4687(3)	1299(2)	37.2(7)
C11	5591.8(13)	6950(3)	2045(2)	38.7(7)
N1	5185.6(8)	1686.4(17)	3678.7(14)	19.7(4)
N2	5220.5(8)	3768.5(17)	3385.9(13)	18.9(4)
C23	6021.0(9)	-1640(2)	5666.1(17)	15.3(5)
C24	6012.5(9)	-3166(2)	5617.4(16)	15.0(4)
C25	6233.7(9)	3275(2)	7195.0(18)	17.7(5)
C26	6233.8(10)	1757(2)	7187.1(18)	17.5(5)
O1	5847.0(7)	-1156.7(13)	6517.9(12)	18.6(3)
O2	6183.4(7)	-1016.4(14)	4928.2(12)	22.6(4)
O3	6075.9(7)	-3679.5(13)	4774.1(11)	20.0(3)
O4	5947.3(6)	-3760.2(13)	6455.7(12)	18.7(3)
O5	6059.0(7)	3796.7(14)	6350.5(11)	22.5(4)
O6	6372.7(9)	3869.3(16)	7948.8(14)	39.1(5)
O7	5856.0(7)	1246.2(14)	6583.3(13)	24.2(4)
O8	6567.9(8)	1179.7(16)	7751.5(14)	34.6(5)

Table 3: Anisotropic Displacement Parameters ($\times 10^4$) for [*i*Bu_2IM](HC_2O_4). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	19.9(11)	18.4(12)	18.5(11)	2(1)	3.0(9)	-0.3(9)
C13	20.5(12)	23.0(12)	25.0(13)	-0.1(10)	6.7(10)	-2.4(9)
C14	18.8(11)	24.1(12)	21.3(12)	-1.5(10)	3.8(10)	1.3(9)
C15	28.0(12)	12.8(11)	31.6(14)	3.4(10)	9.7(10)	0.0(9)
C16	25.1(12)	20.7(12)	39.3(15)	7.6(12)	5.1(11)	-1.6(10)
C17	46.4(17)	33.9(15)	45.5(18)	14.4(14)	12.4(14)	14.3(13)
C18	34.2(15)	29.1(14)	29.6(15)	1.8(12)	-2.4(11)	0.8(11)
C19	25.9(12)	14.5(11)	24.0(13)	-0.1(9)	1(1)	0.6(9)
C20	27.1(12)	24.6(12)	20.2(13)	2.6(10)	2.2(10)	5.5(10)
C21	63(2)	27.9(15)	38.6(17)	11.3(13)	-0.1(16)	8.4(14)
C22	34.1(15)	37.4(15)	23.3(14)	1.8(12)	0.8(11)	7.1(12)
N3	21.4(9)	15.0(9)	22.7(10)	0.8(8)	4.7(8)	0.1(8)
N4	22.5(9)	13.4(9)	18.1(10)	0.7(8)	0.6(8)	-0.6(8)
C1	24.0(11)	16.0(11)	16.3(11)	-1.7(9)	-2.6(9)	-1.8(9)
C2	27.9(13)	21.8(12)	17.2(12)	3.5(9)	-5.9(10)	-5.9(10)
C3	27.9(13)	24.2(13)	16.7(12)	-1(1)	-2.3(10)	-8(1)
C4	33.6(13)	11.6(11)	22.9(12)	1.3(10)	-5.2(11)	-3.8(9)
C5	30.1(13)	21.5(12)	28.2(14)	3.6(11)	-3.8(11)	-4.6(10)
C6	41.0(15)	21.8(13)	37.9(15)	8.9(12)	-8.0(12)	-9.7(11)
C7	36.4(15)	34.4(15)	41.8(17)	1.9(13)	3.0(13)	-4.2(13)
C8	27.3(13)	11.3(11)	27.9(13)	1(1)	-0.7(11)	0.3(9)
C9	24.4(12)	19.5(12)	27.1(13)	4.1(10)	-4.1(11)	-2.4(10)
C10	43.0(16)	35.9(15)	32.6(15)	-0.3(12)	8.9(13)	-0.7(12)
C11	45.8(17)	24.5(14)	45.8(18)	9.0(12)	3.3(14)	-5.4(12)
N1	25.8(10)	16.3(10)	17.0(9)	2.3(8)	-3.0(8)	-2.3(8)
N2	22.1(10)	14.9(9)	19.9(10)	-0.8(8)	-0.4(8)	-2.0(8)
C23	14.2(10)	10.6(10)	21.0(12)	1.9(9)	-1(1)	0.2(9)
C24	11.6(10)	13.8(11)	19.7(12)	0.7(10)	-0.5(9)	-0.6(8)
C25	16.3(10)	14.2(10)	22.6(12)	-0.1(10)	-2.6(9)	-1.3(9)
C26	19.5(11)	14.1(10)	18.8(12)	1(1)	2.4(10)	2.3(9)
O1	28.8(8)	8.9(7)	18.1(8)	-0.3(6)	2.1(7)	-0.3(6)
O2	30.0(9)	12.7(8)	25.0(9)	5.3(7)	7.2(7)	0.6(7)
O3	25.3(8)	14.8(8)	19.8(9)	-3.5(7)	2.2(7)	-2.8(6)
O4	27.2(9)	9.6(7)	19.2(8)	2.2(6)	1.2(7)	-0.7(6)
O5	38.3(10)	9.2(8)	20.1(9)	1.2(7)	-4.0(8)	1.5(7)
O6	67.8(13)	15.8(9)	33.8(11)	0.0(8)	-25.6(10)	-4.4(9)
O7	35.7(9)	8.9(8)	28.1(9)	0.1(7)	-9.9(8)	-0.8(7)
O8	41.8(11)	19.1(9)	42.8(11)	0.7(8)	-20.6(9)	8.6(8)

Table 4. Bond lengths in Å and angles in ° for [*i*Bu_2IM](HC_2O_4).

Atom	Atom	Length/Å
C12	N3	1.329(3)
C12	N4	1.333(3)
C13	C14	1.348(3)
C13	N3	1.380(3)
C14	N4	1.384(3)
C15	C16	1.527(4)
C15	N3	1.474(3)
C16	C17	1.524(3)
C16	C18	1.524(3)
C19	C20	1.527(3)
C19	N4	1.467(3)
C20	C21	1.532(3)
C20	C22	1.520(3)
C1	N1	1.337(3)
C1	N2	1.335(3)
C2	C3	1.349(3)
C2	N1	1.375(3)
C3	N2	1.378(3)

Atom	Atom	Length/Å
C4	C5	1.529(3)
C4	N1	1.474(3)
C5	C6	1.535(3)
C5	C7	1.515(3)
C8	C9	1.522(3)
C8	N2	1.470(3)
C9	C10	1.519(3)
C9	C11	1.527(3)
C23	C24	1.560(3)
C23	O1	1.288(3)
C23	O2	1.219(3)
C24	O3	1.238(3)
C24	O4	1.269(3)
C25	C26	1.550(3)
C25	O5	1.296(3)
C25	O6	1.206(3)
C26	O7	1.278(3)
C26	O8	1.212(3)

Atom	Atom	Atom	Length/Å
N3	C12	N4	108.35(19)
C14	C13	N3	107.23(19)
C13	C14	N4	106.87(19)
N3	C15	C16	112.45(19)
C17	C16	C15	107.6(2)
C18	C16	C15	112.68(19)
C18	C16	C17	111.0(2)
N4	C19	C20	112.56(18)
C19	C20	C21	107.8(2)
C22	C20	C19	111.93(19)
C22	C20	C21	111.9(2)
C12	N3	C13	108.84(18)
C12	N3	C15	125.27(18)
C13	N3	C15	125.81(18)
C12	N4	C14	108.72(17)
C12	N4	C19	125.91(18)
C14	N4	C19	125.30(18)
N2	C1	N1	108.0(2)
C3	C2	N1	107.1(2)
C2	C3	N2	107.3(2)
N1	C4	C5	110.77(19)
C4	C5	C6	109.1(2)
C7	C5	C4	112.1(2)
C7	C5	C6	111.3(2)

Atom	Atom	Atom	Length/Å
N2	C8	C9	112.26(18)
C8	C9	C11	108.82(19)
C10	C9	C8	111.4(2)
C10	C9	C11	111.4(2)
C1	N1	C2	108.91(18)
C1	N1	C4	126.77(19)
C2	N1	C4	124.24(19)
C1	N2	C3	108.70(18)
C1	N2	C8	127.42(19)
C3	N2	C8	123.86(19)
O1	C23	C24	114.51(18)
O2	C23	C24	119.51(19)
O2	C23	O1	125.98(19)
O3	C24	C23	117.30(18)
O3	C24	O4	126.42(19)
O4	C24	C23	116.28(18)
O5	C25	C26	113.91(19)
O6	C25	C26	120.6(2)
O6	C25	O5	125.50(19)
O7	C26	C25	114.35(19)
O8	C26	C25	118.8(2)
O8	C26	O7	126.8(2)

Table 5: Torsion Angles in ° for [*i*Bu$_2$IM](HC$_2$O$_4$).

Atom	Atom	Atom	Atom	Angle/°
C13	C14	N4	C12	0.0(3)
C13	C14	N4	C19	-177.1(2)
C14	C13	N3	C12	0.3(3)
C14	C13	N3	C15	-176.6(2)
C16	C15	N3	C12	-86.9(3)
C16	C15	N3	C13	89.4(3)
C20	C19	N4	C12	-108.8(2)
C20	C19	N4	C14	67.8(3)
N3	C12	N4	C14	0.2(3)
N3	C12	N4	C19	177.23(19)
N3	C13	C14	N4	-0.2(3)
N3	C15	C16	C17	-178.78(19)
N3	C15	C16	C18	-56.1(3)
N4	C12	N3	C13	-0.3(3)
N4	C12	N3	C15	176.60(19)
N4	C19	C20	C21	-173.8(2)
N4	C19	C20	C22	62.7(3)
C2	C3	N2	C1	-0.3(3)
C2	C3	N2	C8	-178.8(2)
C3	C2	N1	C1	-0.6(3)
C3	C2	N1	C4	-177.6(2)
C5	C4	N1	C1	-115.7(3)
C5	C4	N1	C2	60.7(3)
C9	C8	N2	C1	-102.4(2)
C9	C8	N2	C3	75.8(3)
N1	C1	N2	C3	-0.1(3)
N1	C1	N2	C8	178.35(19)
N1	C2	C3	N2	0.6(3)
N1	C4	C5	C6	-173.66(19)
N1	C4	C5	C7	62.6(3)
N2	C1	N1	C2	0.4(3)
N2	C1	N1	C4	177.3(2)
N2	C8	C9	C10	69.9(3)
N2	C8	C9	C11	-166.9(2)
O1	C23	C24	O3	167.92(19)
O1	C23	C24	O4	-12.8(3)
O2	C23	C24	O3	-11.9(3)
O2	C23	C24	O4	167.30(19)
O5	C25	C26	O7	-27.7(3)
O5	C25	C26	O8	154.2(2)
O6	C25	C26	O7	150.5(2)
O6	C25	C26	O8	-27.6(3)

Table 6. Hydrogen Atom Coordinates (Åx10^4) and Isotropic Displacement Parameters (Å^2 x 10^3) for [*i*Bu_2IM](HC_2O_4). U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

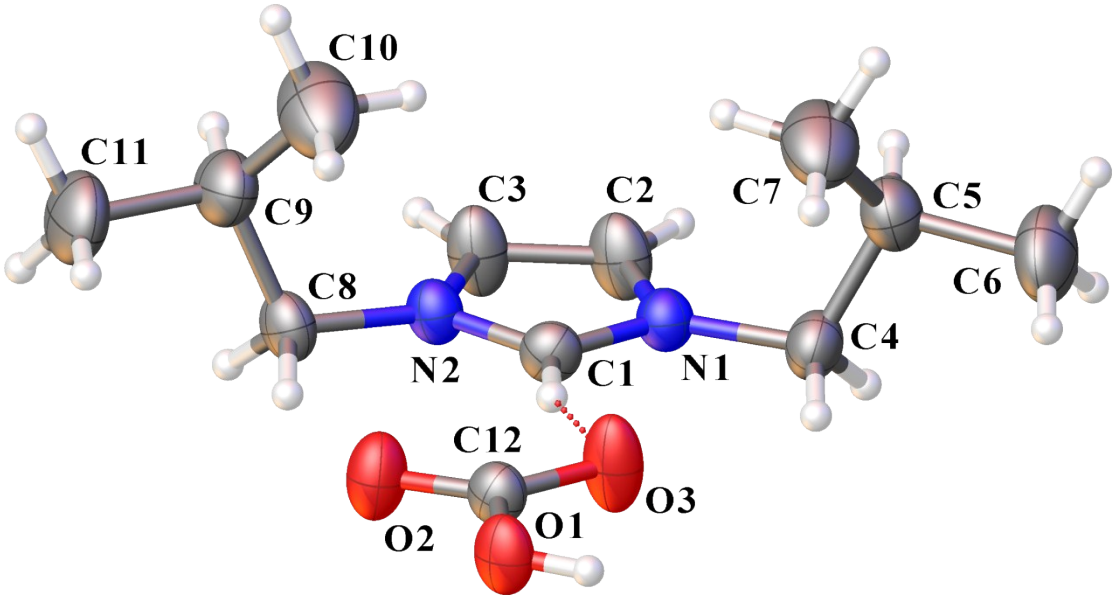
Atom	x	y	z	U_{eq}
H12	6760	7401	3922	23
H13	8303	8598	2736	27
H14	8361	6196	2978	26
H15A	7538	10417	3345	29
H15B	6930	9924	3843	29
H16	6531	9459	2239	34
H17A	7014	12052	2314	63
H17B	6426	11605	2899	63
H17C	6436	11642	1686	63
H18A	7638	10303	1404	46
H18B	7058	10049	735	46
H18C	7370	8857	1314	46
H19A	7425	4407	3280	26
H19B	6921	4962	4017	26
H20	8136	4636	4608	29
H21A	7783	2792	5545	65
H21B	7682	2596	4354	65
H21C	7138	3000	5066	65
H22A	7674	6299	5563	47
H22B	7818	5070	6275	47
H22C	7156	5309	5881	47
H1	4693	2543	2558	22
H2	5787	1756	4878	27
H3	5835	4139	4533	28
H4A	5373	-251	3538	27
H4B	4740	141	3080	27
H5	4998	90	5213	32
H6A	4468	-1880	5300	50
H6B	4986	-2050	4481	50
H6C	4318	-1813	4115	50
H7A	4223	1572	4783	56
H7B	3998	420	5510	56
H7C	3853	374	4322	56
H8A	5084	5722	3497	27
H8B	4762	5074	2539	27
H9	6024	5339	2650	28
H10A	5704	3756	1468	56
H10B	6007	4961	890	56
H10C	5301	4828	913	56
H11A	5931	7234	1637	58
H11B	5585	7439	2684	58
H11C	5224	7113	1670	58
H5A	6009(11)	4810(30)	6410(20)	34
H1A	5855(15)	90(40)	6580(30)	85(11)

Table 7: Hydrogen Bond information for [*i*Bu_2IM](HC_2O_4).

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O5	H5A	O4[1]	1.04(3)	1.47(3)	2.5112(19)	178(3)
O7	H1A	O1	1.18(4)	1.28(4)	2.4552(19)	177(4)
C1	H1	O1[2]	0.95	2.32	3.167(3)	148.6
C1	H1	O4[2]	0.95	2.40	3.202(3)	142.4

[1]+x,1+y,+z, [2]1-x,-y,-1/2+z

Crystal structure of [*i*Bu$_2$IM](HCO$_3$) - view 1 with labelled atoms



Crystal structure of [*i*Bu$_2$IM](HCO$_3$) - view 2

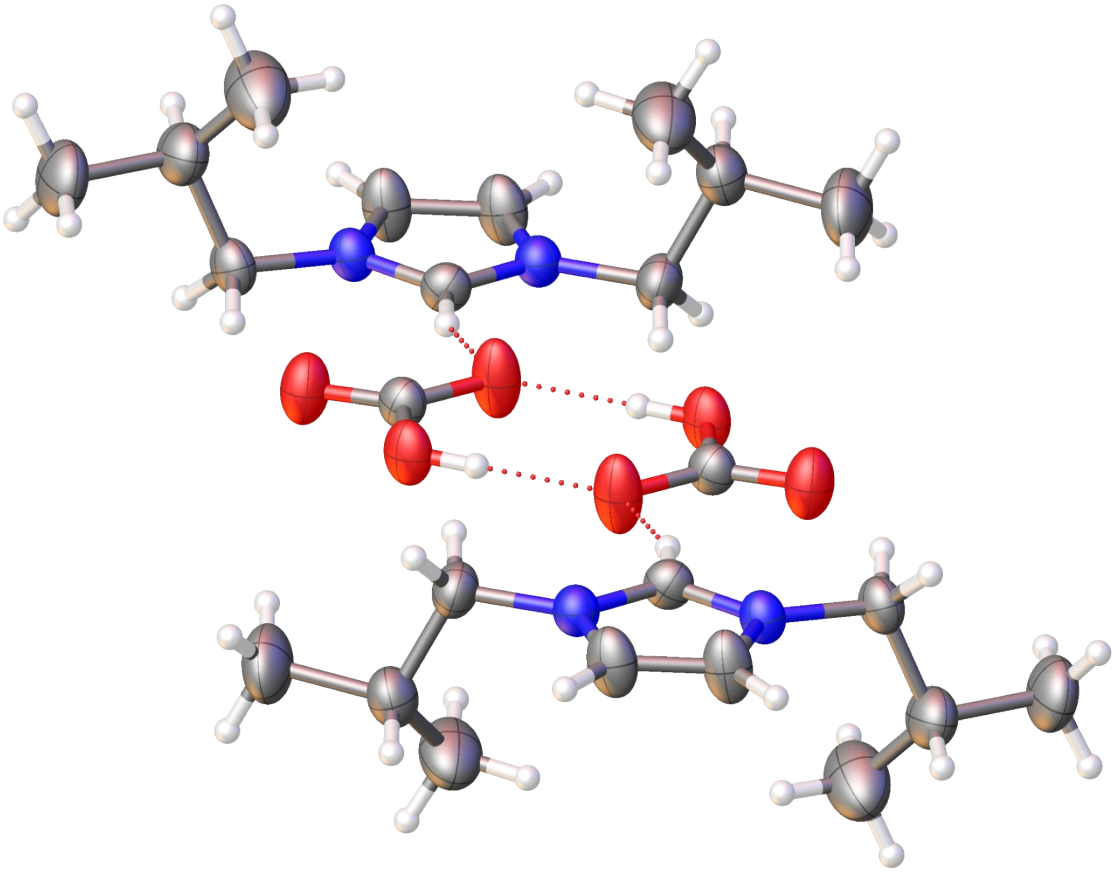


Table 8. Crystal data and structure refinement for [*i*Bu_2IM](HCO_3)

CCDC	1560698
Formula	$C_{12}H_{22}N_2O_3$
$D_{calc.}$ / g cm^{-3}	1.106
μ / mm^{-1}	0.079
Formula Weight	242.31
Colour	colourless
Shape	prism
Size / mm^3	0.55 × 0.50 × 0.50
T / K	298
Crystal System	monoclinic
Space Group	$P2_1/n$
a / Å	10.1801(12)
b / Å	12.3007(15)
c / Å	11.6842(15)
α / °	90
β / °	96.132(4)
γ / °	90
V = $Å^3$	1454.8(3)
Z	4
Θ_{min} / °	2.411
Θ_{max} / °	27.665
Measured Refl.	31087
Independent Refl.	3369
Reflections Used	1961
R_{int}	0.0348
Parameters	159
Restraints	0
Largest Peak Largest Peak	0.527
Deepest Hole	-0.222
GooF	1.017
ωR_2 (all data)	0.2294
ωR_2	0.1815
R_1 (all data)	0.1170
R_1	0.0679

Table 9. Fractional atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^{2}x10^3) for [*i*Bu_2IM](HCO_3). *U(eq)* is defined as one third of the trace of the orthogonalized *Uij* tensor.

Atom	x	y	z	U(eq)
O1	3398.0(17)	282.3(16)	5437.1(17)	71.9(6)
N2	3601.9(19)	3459.7(17)	1947.5(17)	55.9(5)
N1	5490.8(19)	2743.3(17)	1749.3(17)	56.4(5)
O2	2587(2)	1622.3(18)	4359.3(18)	84.2(7)
O3	4608(2)	1029.1(19)	4197(2)	92.9(8)
C1	4434(2)	2679(2)	2298(2)	57.1(6)
C12	3540(2)	1025(2)	4633(2)	56.9(6)
C8	2335(2)	3662(2)	2397(2)	63.6(7)
C4	6651(3)	2032(2)	1916(3)	70.0(7)
C2	5329(3)	3599(3)	1005(3)	78.6(9)
C5	7826(3)	2536(3)	2605(3)	78.2(8)
C3	4160(3)	4048(3)	1130(3)	80.4(9)
C9	2371(3)	4622(3)	3184(3)	88(1)
C11	1030(4)	4714(4)	3655(4)	112.9(14)
C6	8967(3)	1727(4)	2671(4)	117.3(14)
C7	7535(4)	2892(4)	3764(4)	123.7(16)
C10	3474(4)	4603(5)	4102(4)	138.8(19)

Table 10: Anisotropic Displacement Parameters (×10^4) for [*i*Bu_2IM](HCO_3). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	61.3(11)	83.3(13)	76.5(12)	25.6(10)	32.1(9)	6.3(9)
N2	50.8(10)	64.2(12)	54.3(11)	10.4(9)	13.4(8)	0.7(9)
N1	53.0(11)	61.5(12)	55.8(12)	4.1(10)	10.8(9)	2.0(9)
O2	75.6(13)	91.7(15)	89.7(15)	26.9(12)	28.7(11)	24.5(11)
O3	71.0(12)	101.5(16)	114.2(17)	60.7(13)	46.8(12)	21.8(11)
C1	62.2(14)	54.7(13)	56.5(14)	8.4(11)	15.6(11)	-2.9(11)
C12	56.4(14)	59.9(14)	56.9(14)	6.4(12)	18.2(11)	-1.5(11)
C8	49.2(13)	79.2(17)	65.1(15)	8.8(13)	18.2(11)	-0.2(12)
C4	62.9(16)	71.0(17)	77.1(18)	-5.6(14)	11.3(13)	14.2(13)
C2	63.6(16)	104(2)	72.5(18)	32.7(17)	27.2(13)	7.7(15)
C5	62.0(16)	87(2)	86(2)	6.2(16)	7.8(14)	5.5(14)
C3	64.5(16)	101(2)	79.6(19)	45.6(17)	25.1(14)	16.1(15)
C9	73.4(19)	99(2)	95(2)	-14.3(19)	28.4(17)	4.9(17)
C11	89(2)	134(3)	123(3)	-15(3)	47(2)	22(2)
C6	78(2)	149(4)	122(3)	-9(3)	-4(2)	40(2)
C7	94(3)	163(4)	110(3)	-47(3)	-9(2)	12(3)
C10	105(3)	201(5)	111(3)	-56(3)	16(3)	7(3)

Table 11. Bond lengths in Å and angles in ° for [*i*Bu$_2$IM](HCO$_3$).

Atom	Atom	Length/ Å	Atom	Atom	Length/ Å
O1	C12	1.330(3)	O3	C12	1.248(3)
N2	C1	1.317(3)	C8	C9	1.495(4)
N2	C8	1.465(3)	C4	C5	1.502(4)
N2	C3	1.369(3)	C2	C3	1.334(4)
N1	C1	1.312(3)	C5	C6	1.524(5)
N1	C4	1.466(3)	C5	C7	1.482(5)
N1	C2	1.364(3)	C9	C11	1.531(4)
O2	C12	1.232(3)	C9	C10	1.467(6)

Atom	Atom	Atom	Angle/ °	Atom	Atom	Atom	Angle/ °
C1	N2	C8	125.0(2)	N2	C8	C9	112.9(2)
C	N2	C3	107.5(2)	N1	C4	C5	114.1(2)
C3	N2	C8	127.4(2)	C3	C2	N1	107.4(2)
C1	N1	C4	126.1(2)	C4	C5	C6	108.5(3)
C1	N1	C2	108.0(2)	C7	C5	C4	112.7(3)
C2	N1	C4	125.9(2)	C7	C5	C6	111.9(3)
N1	C1	N2	109.7(2)	C2	C3	N2	107.4(2)
O2	C12	O1	116.8(2)	C8	C9	C11	108.4(3)
O2	C12	O3	126.0(2)	C10	C9	C8	113.9(3)
O3	C12	O1	117.1(2)	C10	C9	C11	112.4(3)

Table 12: Torsion Angles in ° for for [*i*Bu$_2$IM](HCO$_3$).

Atom	Atom	Atom	Atom	Angle/°
N2	C8	C9	C11	-176.7(3)
N2	C8	C9	C10	-50.8(4)
N1	C4	C5	C6	-177.9(3)
N1	C4	C5	C7	57.7(4)
N1	C2	C3	N2	-0.4(4)
C1	N2	C8	C9	104.5(3)
C1	N2	C3	C2	0.1(4)
C1	N1	C4	C5	-103.2(3)
C1	N1	C2	C3	0.5(4)
C8	N2	C1	N1	-178.0(2)
C8	N2	C3	C2	178.2(3)
C4	N1	C1	N2	178.7(2)
C4	N1	C2	C3	-178.7(3)
C2	N1	C1	N2	-0.4(3)
C2	N1	C4	C5	75.8(4)
C3	N2	C1	N1	0.2(3)
C3	N2	C8	C9	-73.3(4)

Table 13. Hydrogen Atom Coordinates (Åx10^4) and Isotropic Displacement Parameters (Å^2 x 10^3) for [*i*Bu_2IM](HCO_3).

Atom	x	y	z	U(eq)
H1A	4041	-123	5498	108
H1	4294	2160	2852	69
H8A	2088	3022	2810	76
H8B	1661	3779	1757	76
H4A	6901	1826	1168	84
H4B	6412	1374	2301	84
H2	5924	3827	504	94
H5	8085	3178	2187	94
H3	3792	4649	734	96
H9	2479	5270	2716	106
H11A	340	4727	3027	169
H11B	1001	5373	4093	169
H11C	905	4102	4141	169
H6A	8703	1060	3006	176
H6B	9714	2025	3137	176
H6C	9202	1588	1910	176
H7A	6852	3434	3687	186
H7B	8318	3193	4174	186
H7C	7245	2280	4180	186
H10A	3372	3998	4603	208
H10B	3479	5267	4535	208
H10C	4291	4534	3768	208

Table 14: Hydrogen Bond information for for [*i*Bu_2IM](HCO_3).

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1	H1A	O3[1]	0.82	1.78	2.593(3)	173.1
C1	H1	O3	0.93	2.10	2.997(3)	162.5

[1]1-x,-y,1-z

References

[1] APEX2 suite for crystallographic software: Bruker V8.34A: SADABS, SAINT, APEX2. Bruker AXS Inc Bruker axs, Madison, WI (2014).

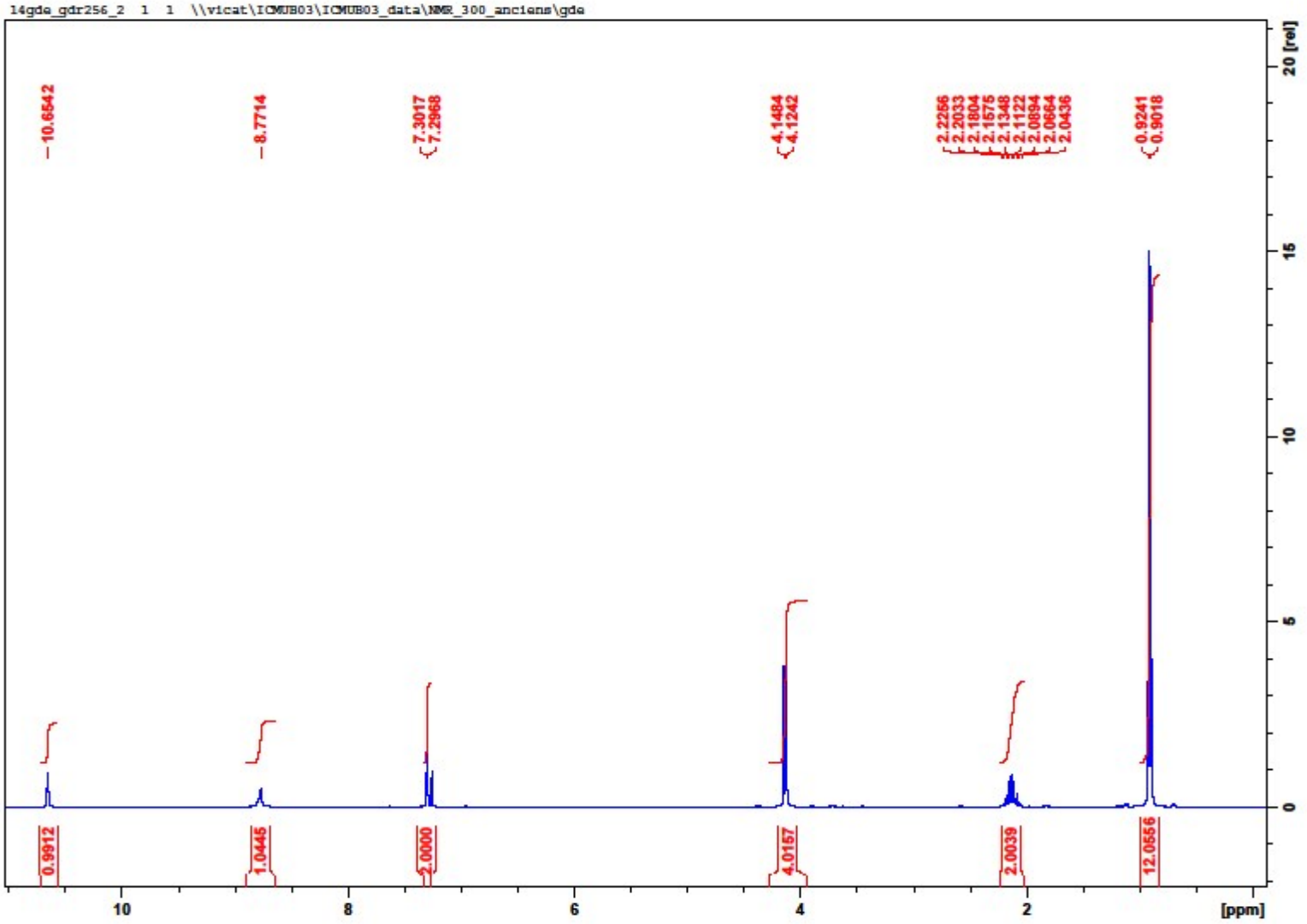
[2] Sheldrick, G. M. Acta Cryst. (2008) **A64**, 112-12.

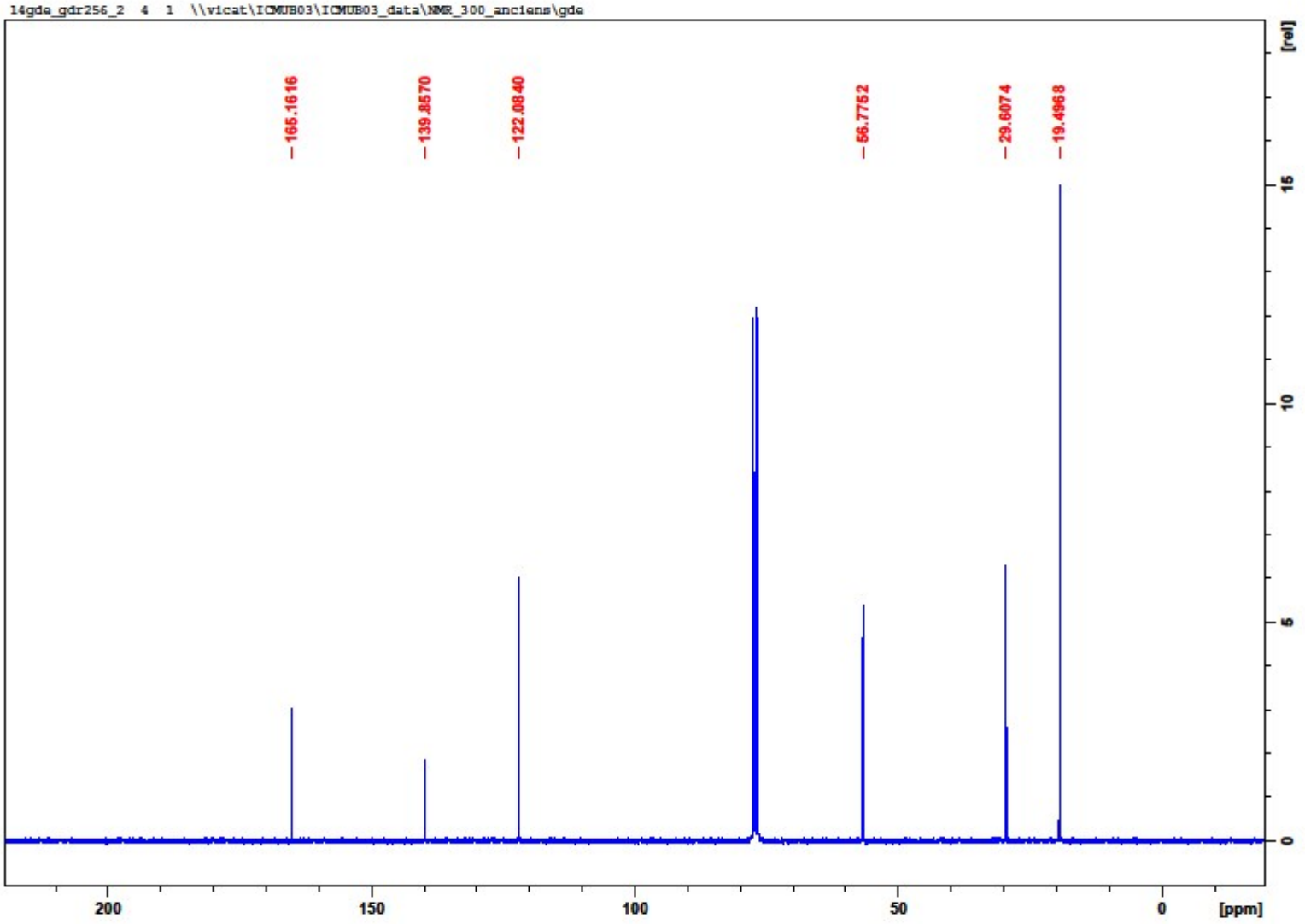
[3] O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.

^{1}H and ^{13}C NMR spectra for imidazolium salts

Experiments of CO_2 chemisorption:

[*i*Bu$_2$IM](HC$_2$O$_4$)

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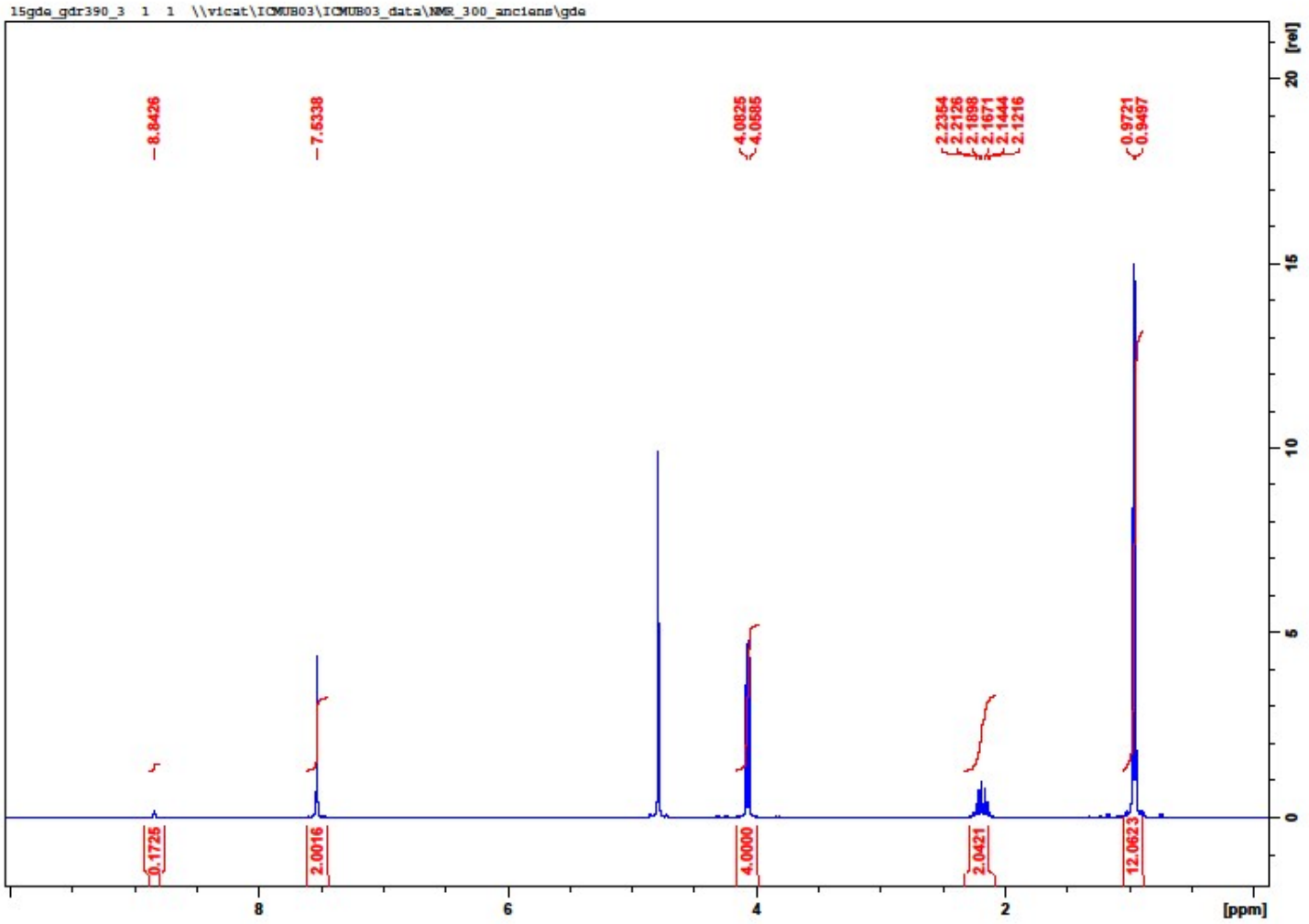
[*i*Bu$_2$IM](HCO$_3$)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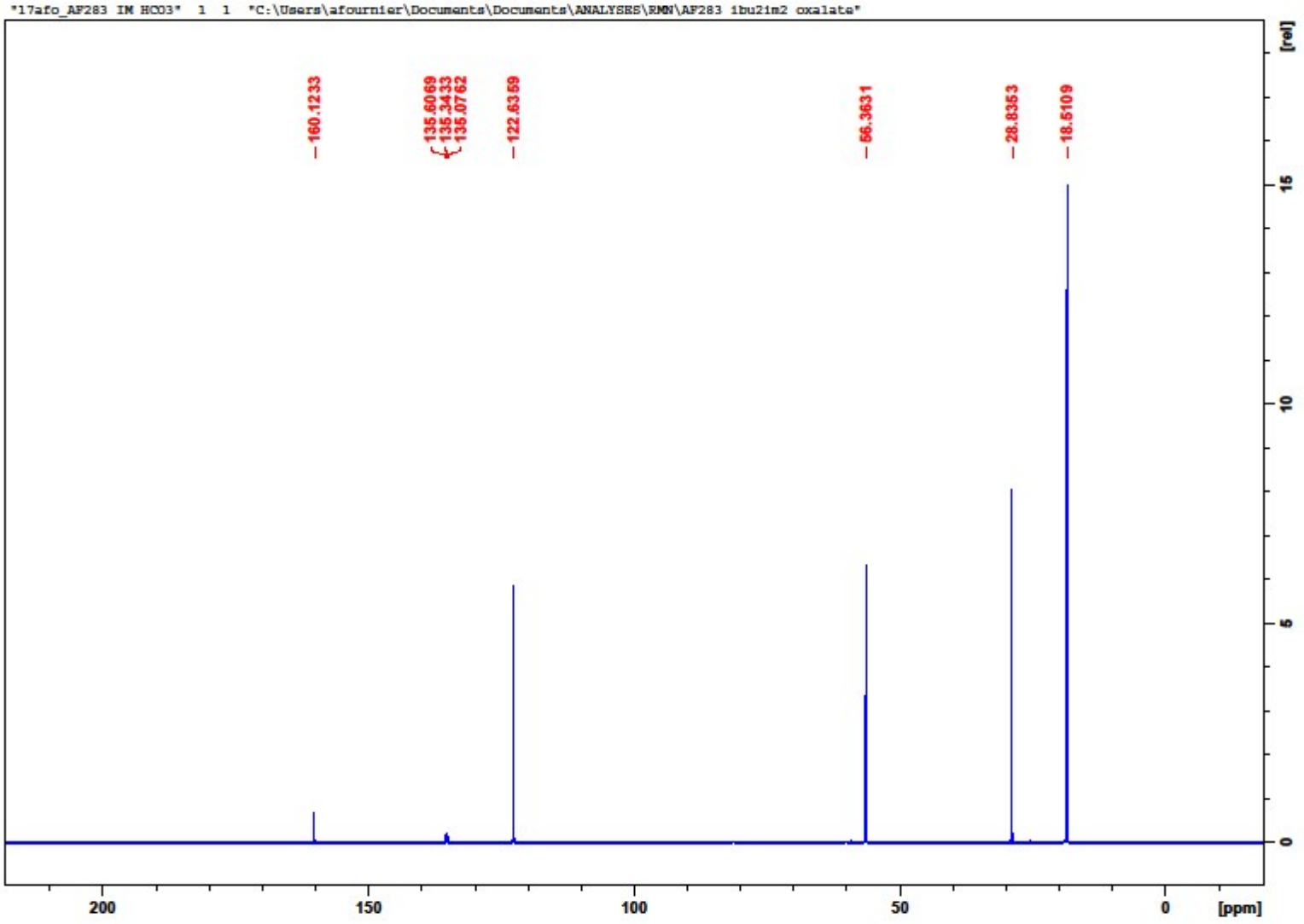
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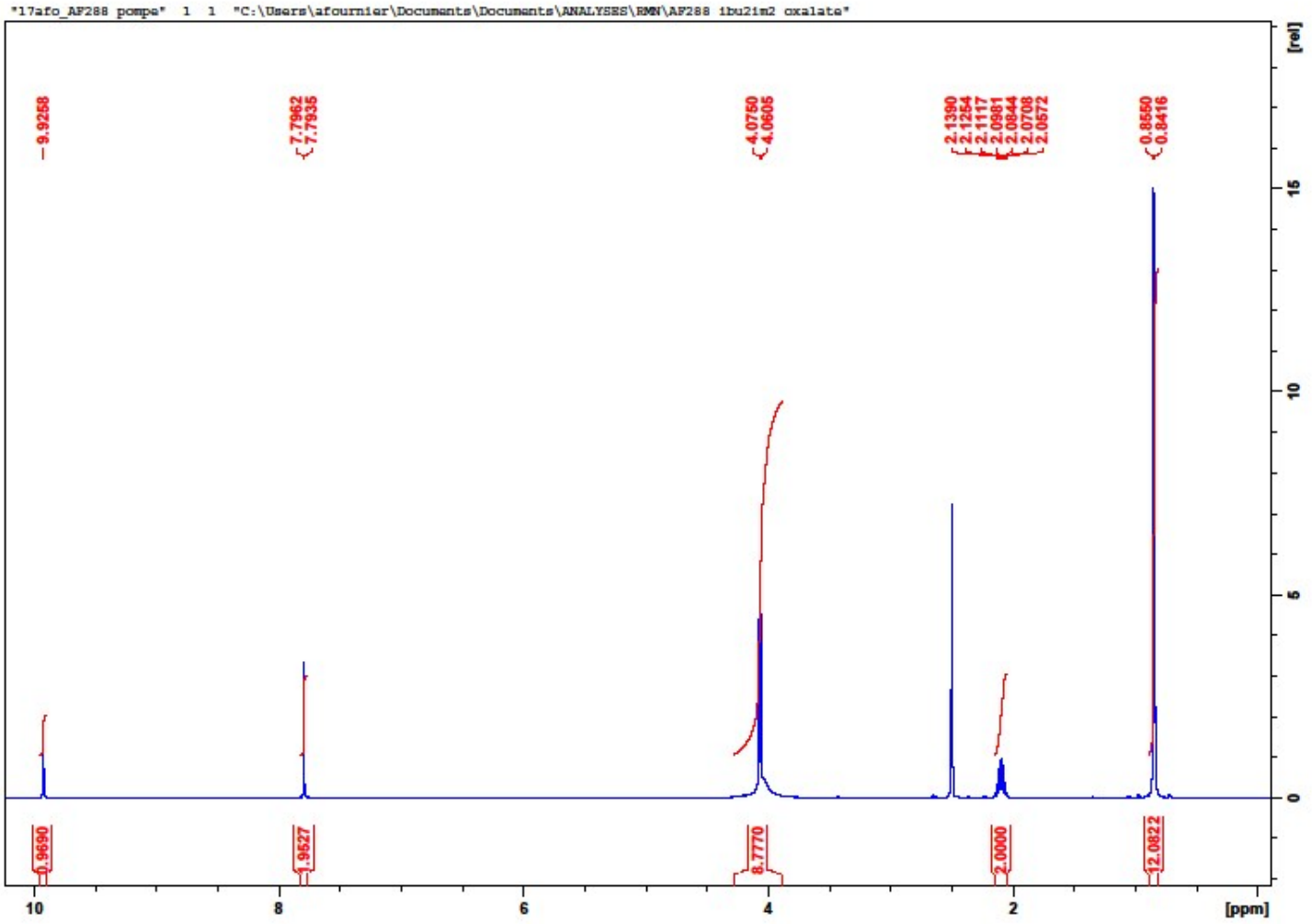
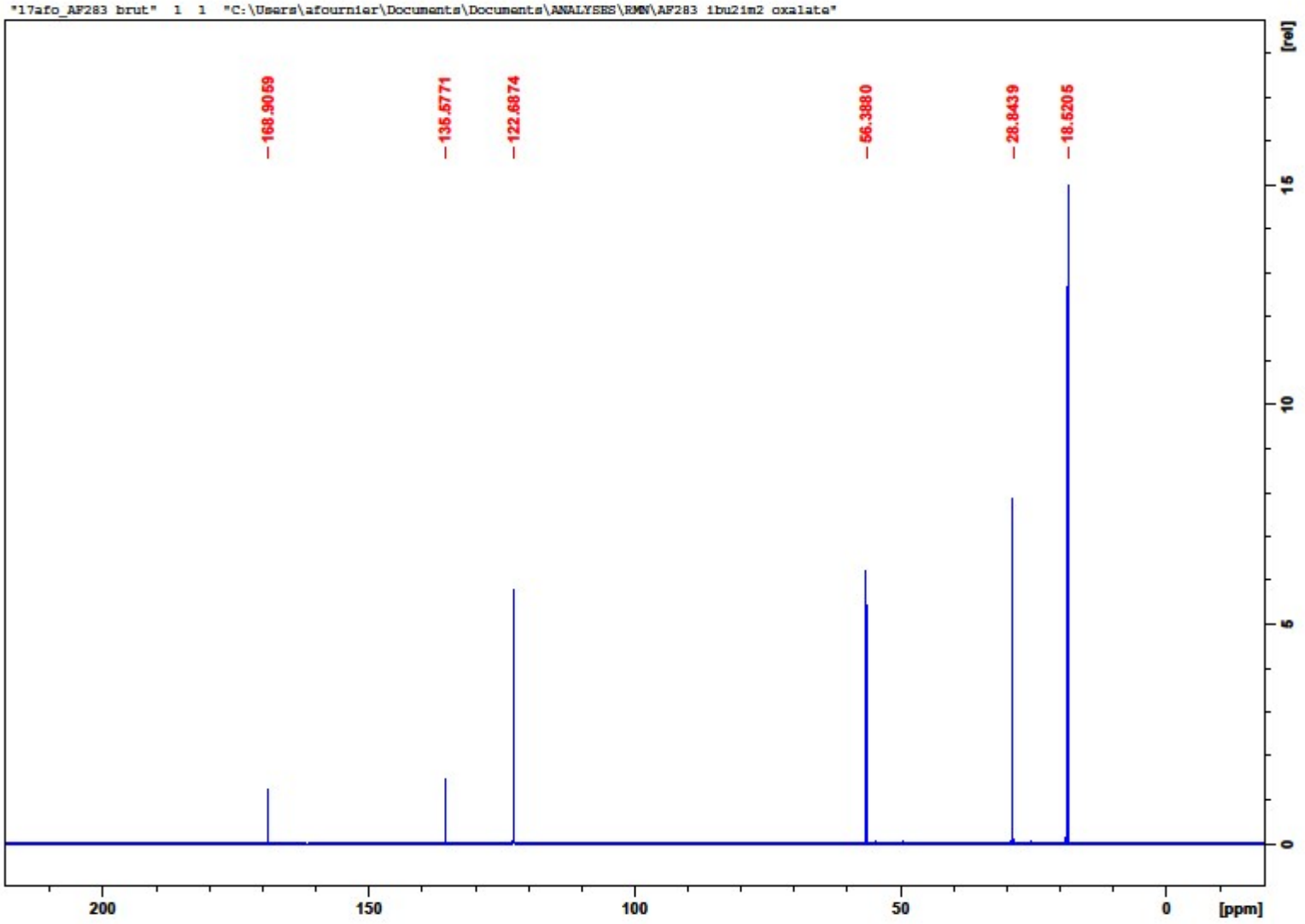
[*i*Bu$_2$IM]$_2$(C$_2$O$_4$)

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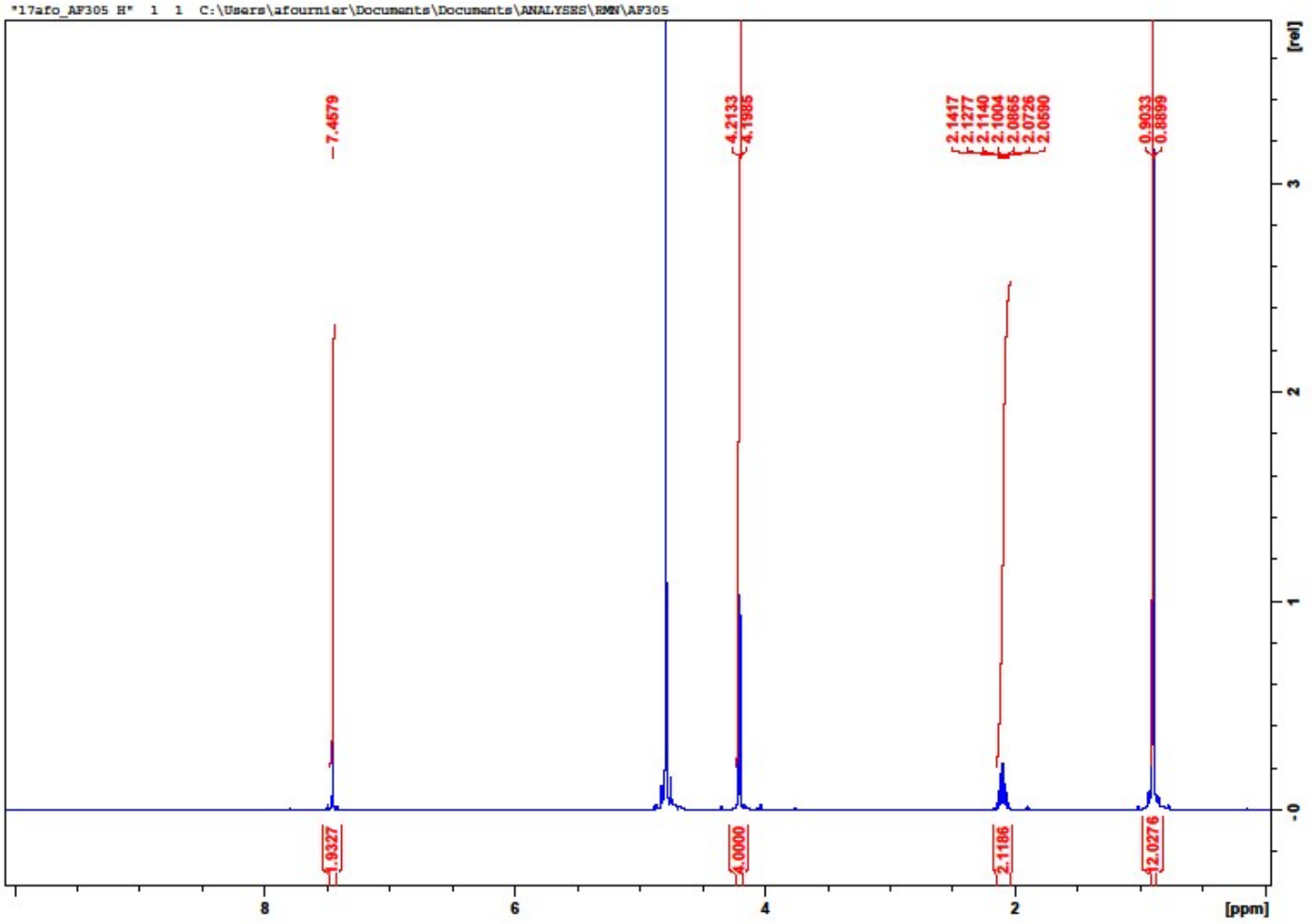
[*i*Bu$_2$IM](CO$_2$)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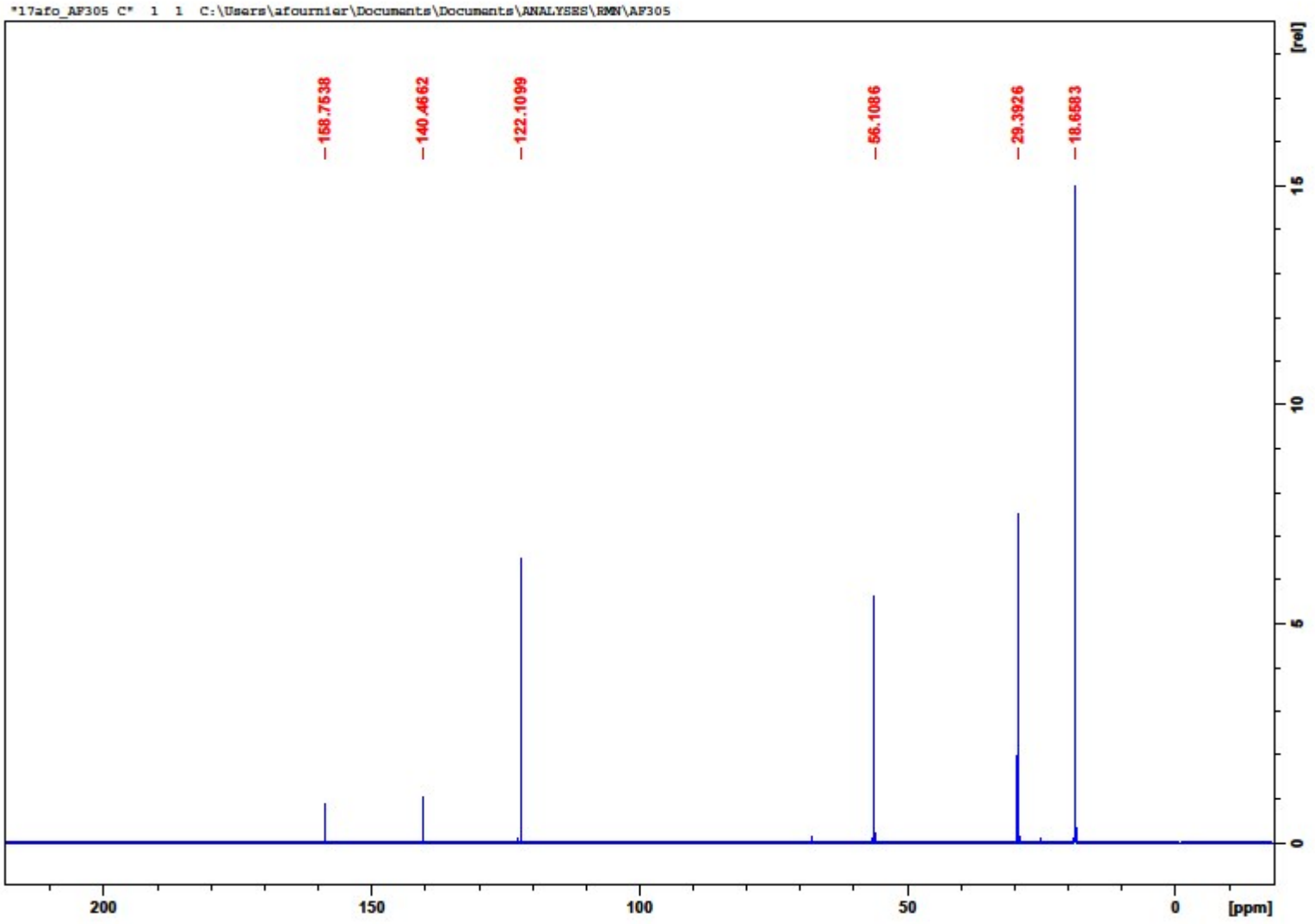
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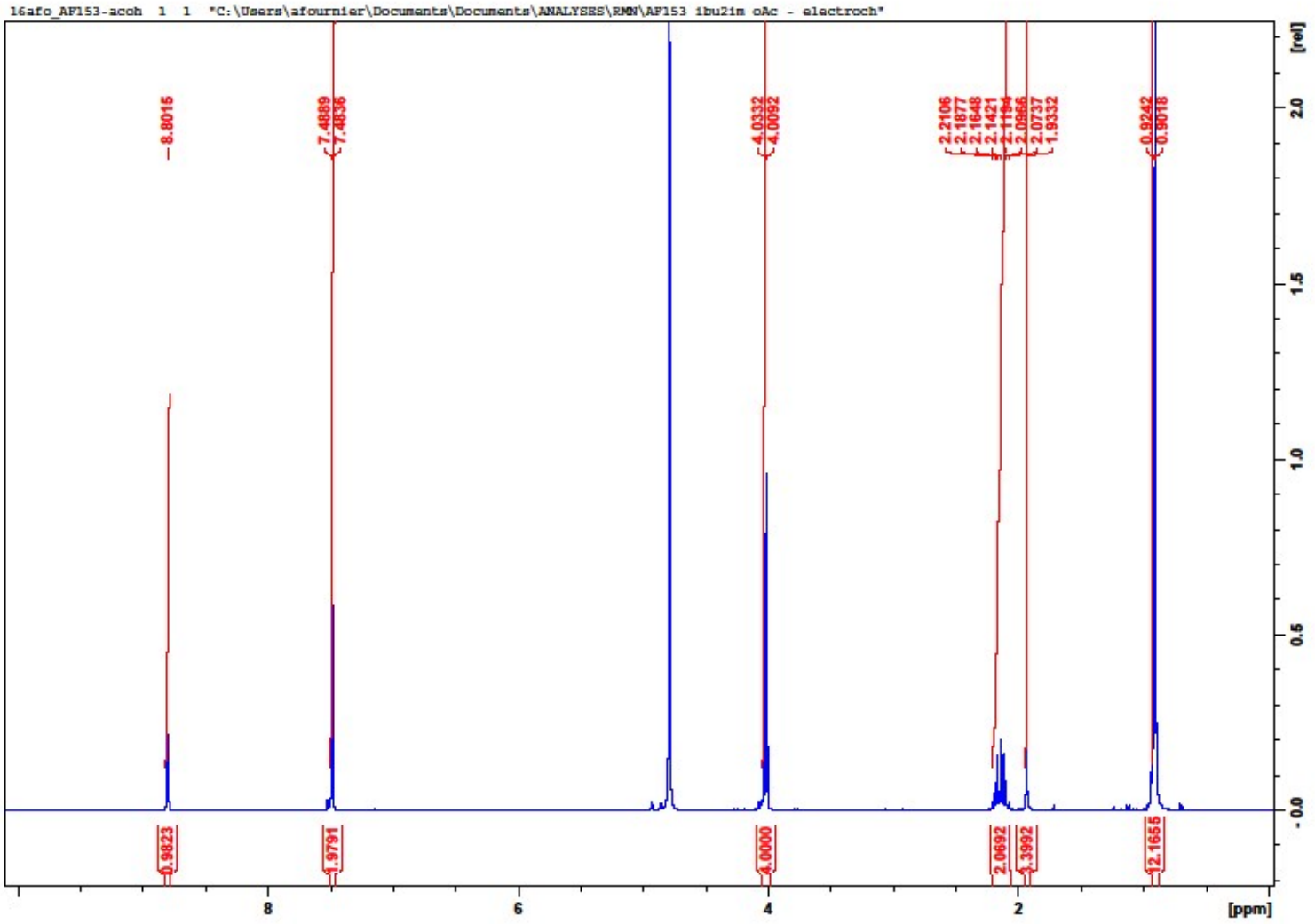
[*i*Bu$_2$IM](OAc)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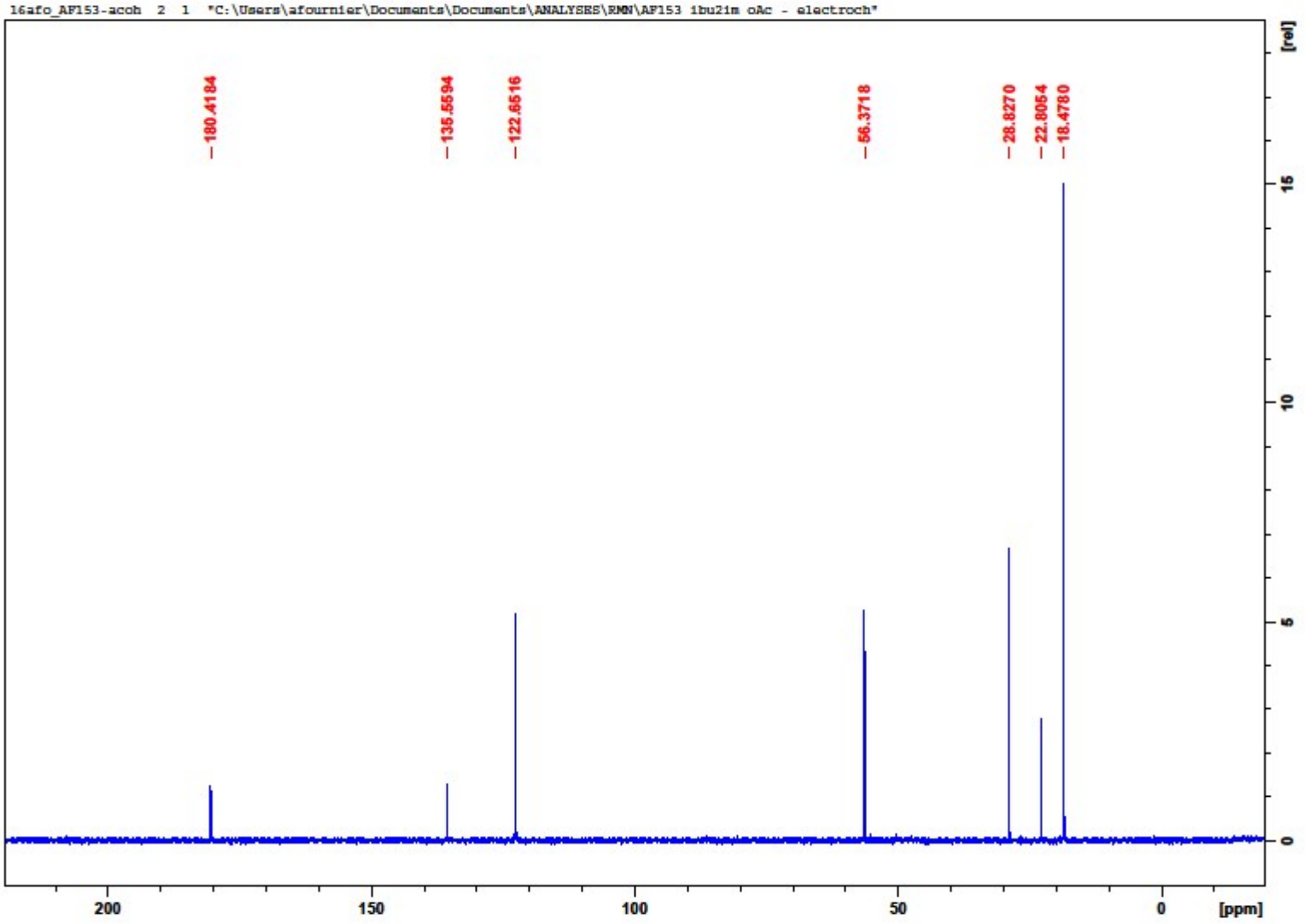
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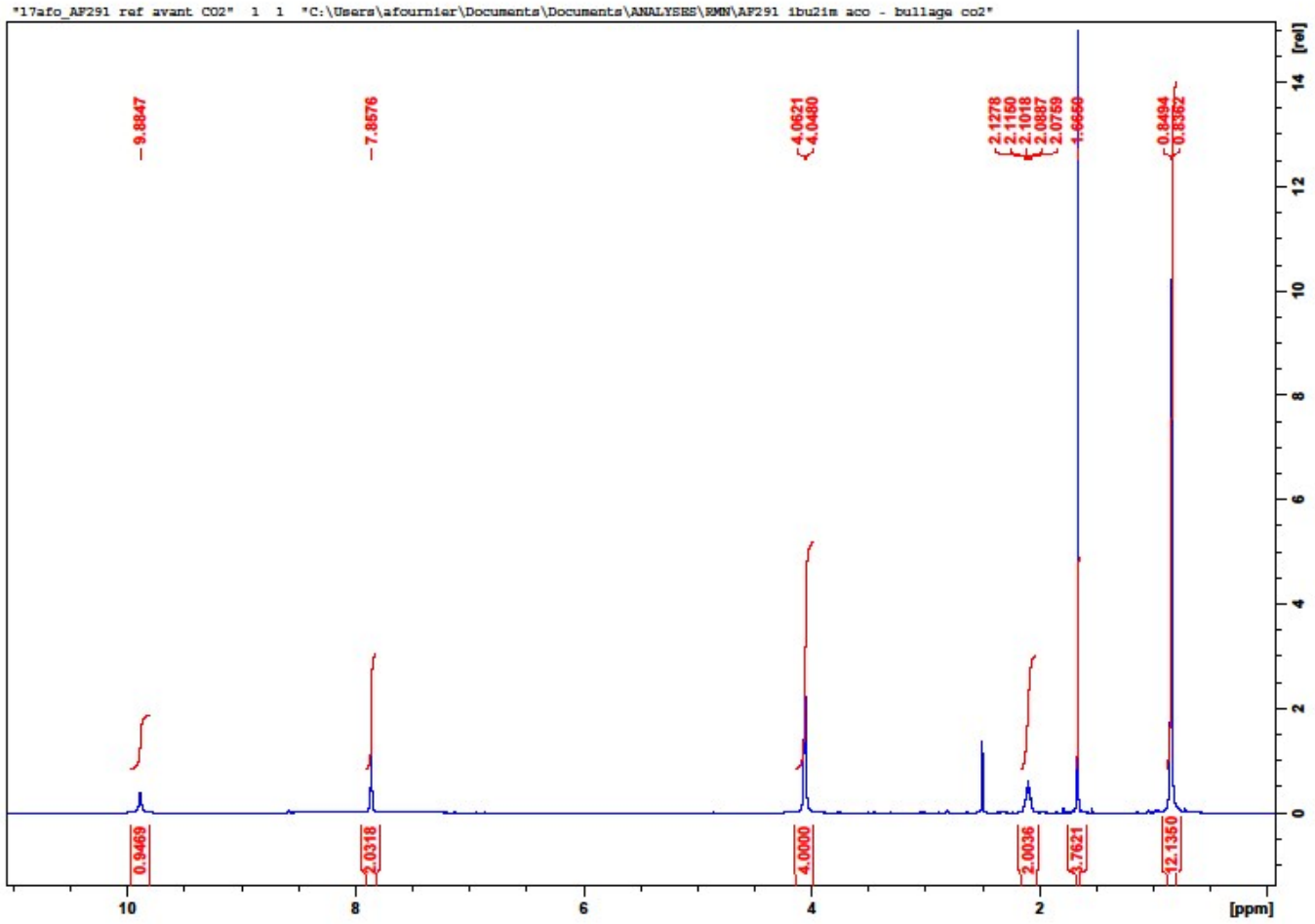
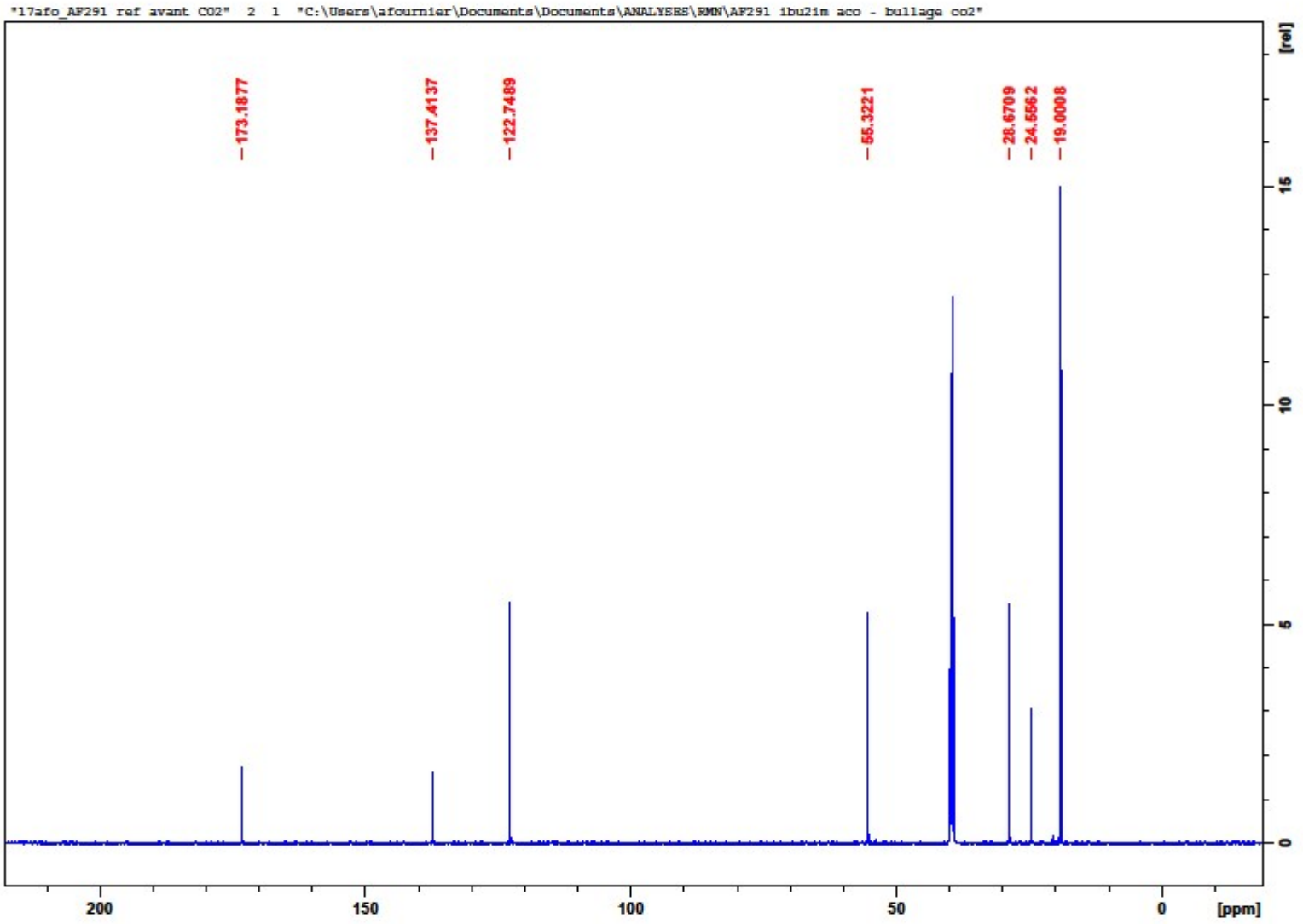
Experiments of CO_2 chemisorption with [*i*Bu_2IM](OAc)

Before CO_2 bubbling

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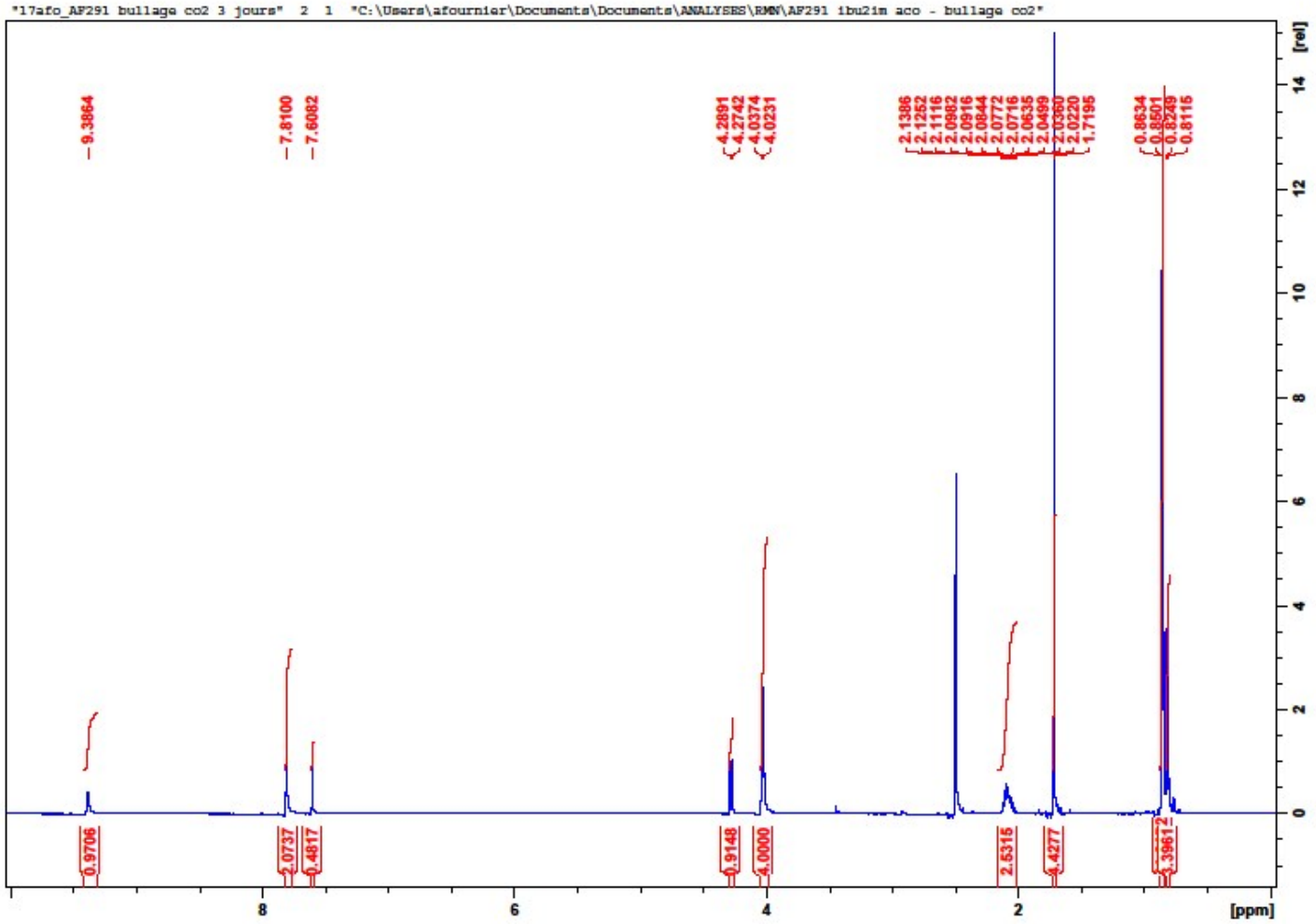
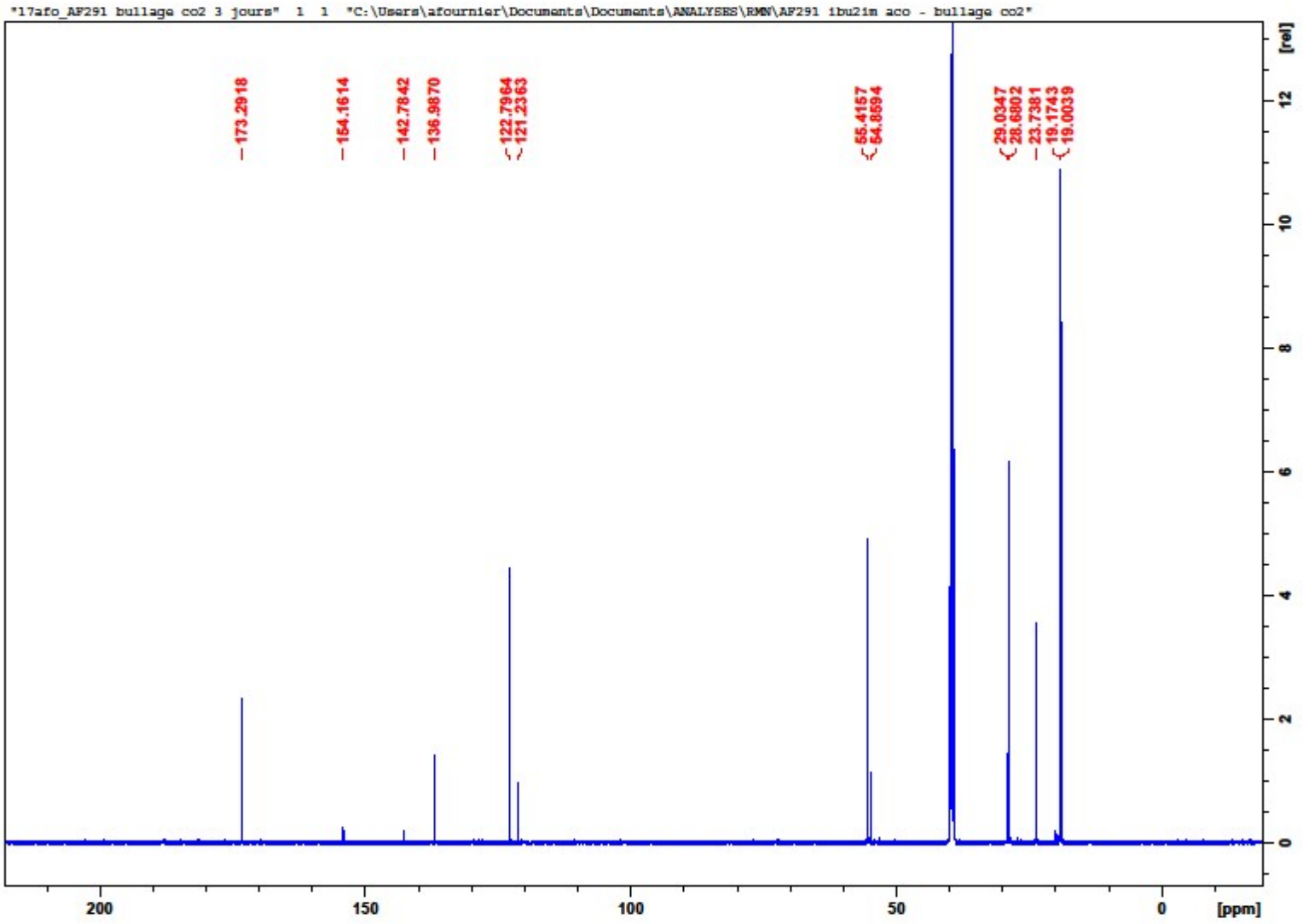
After CO_2 bubbling

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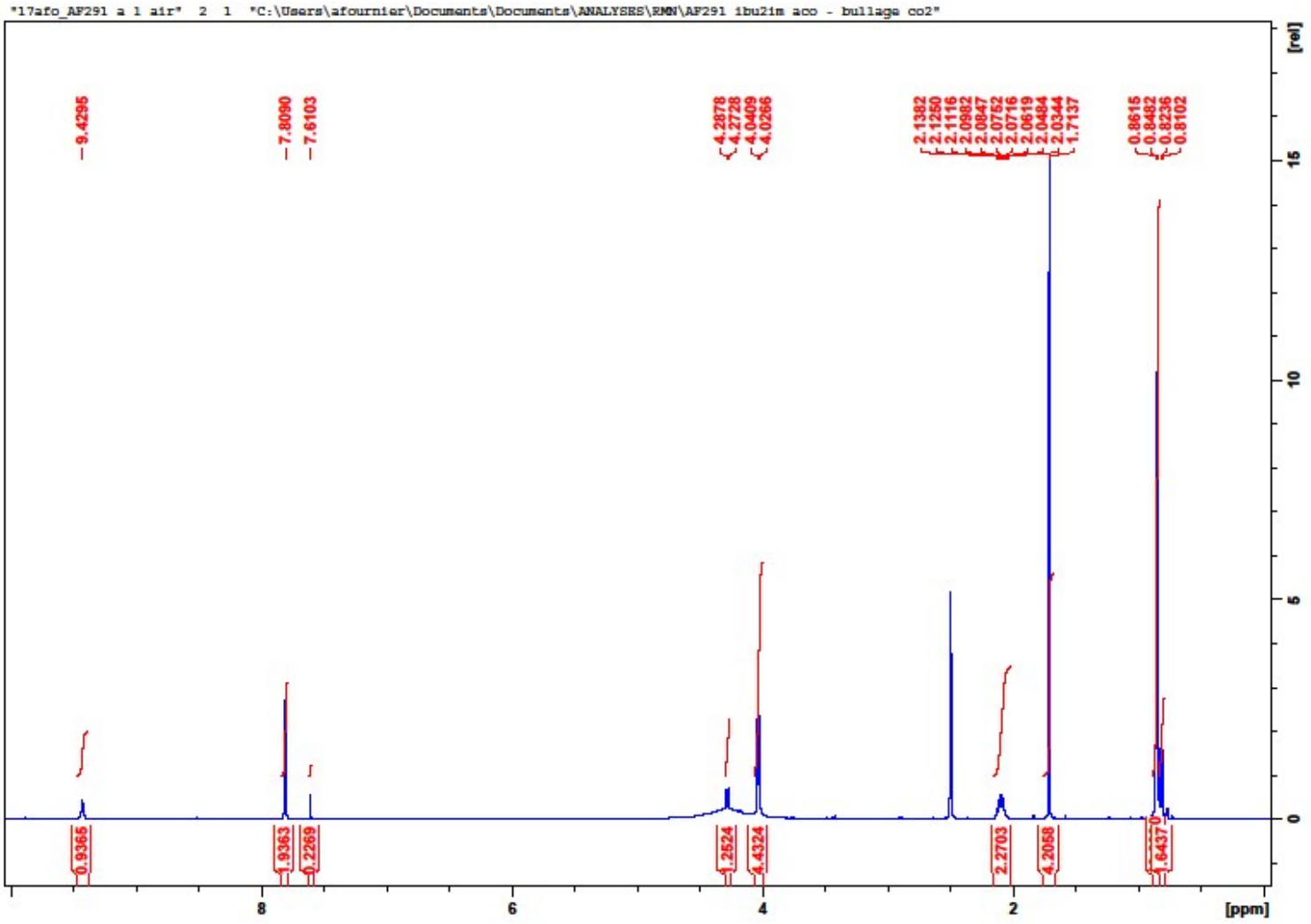
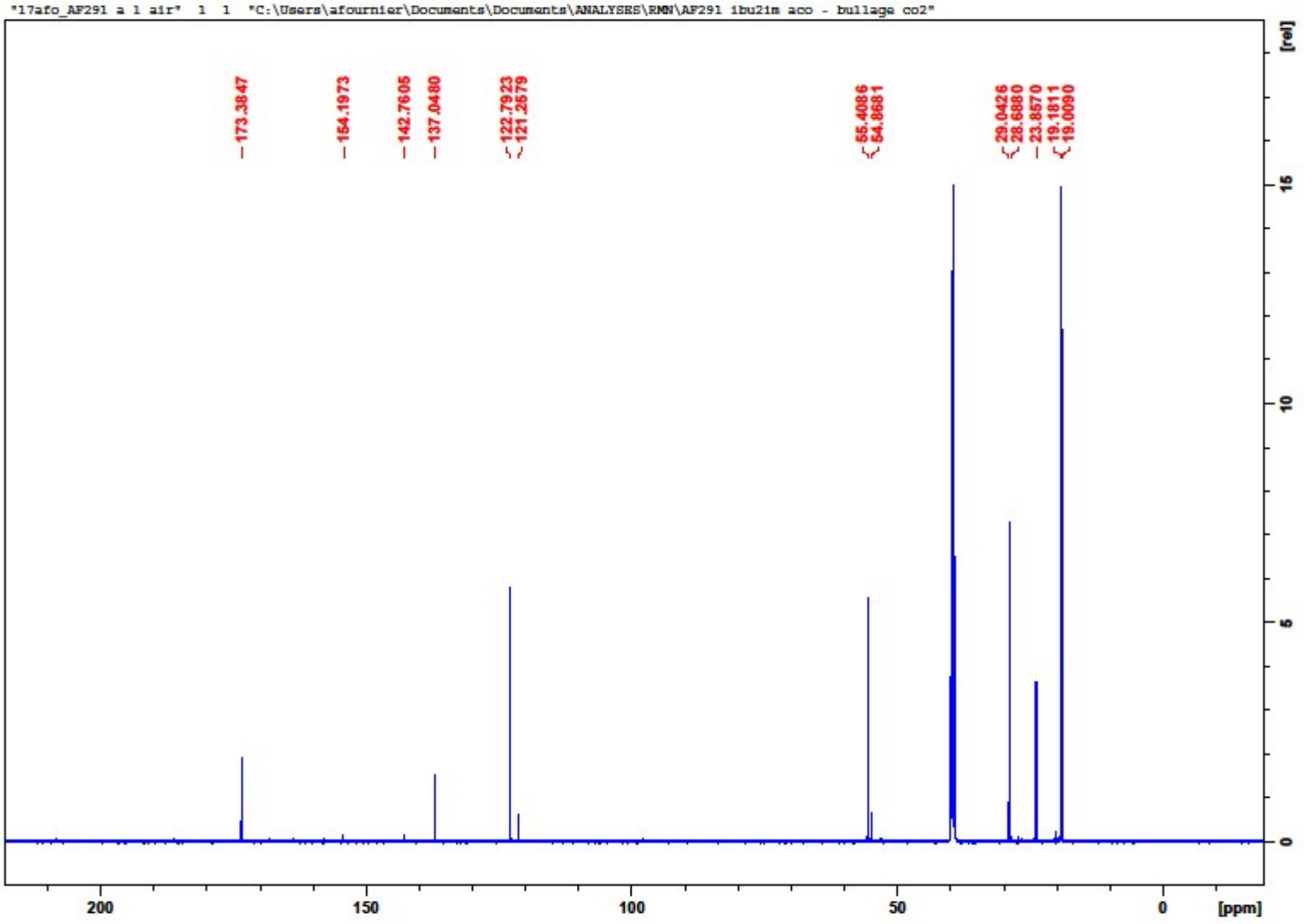
NMR sample open air

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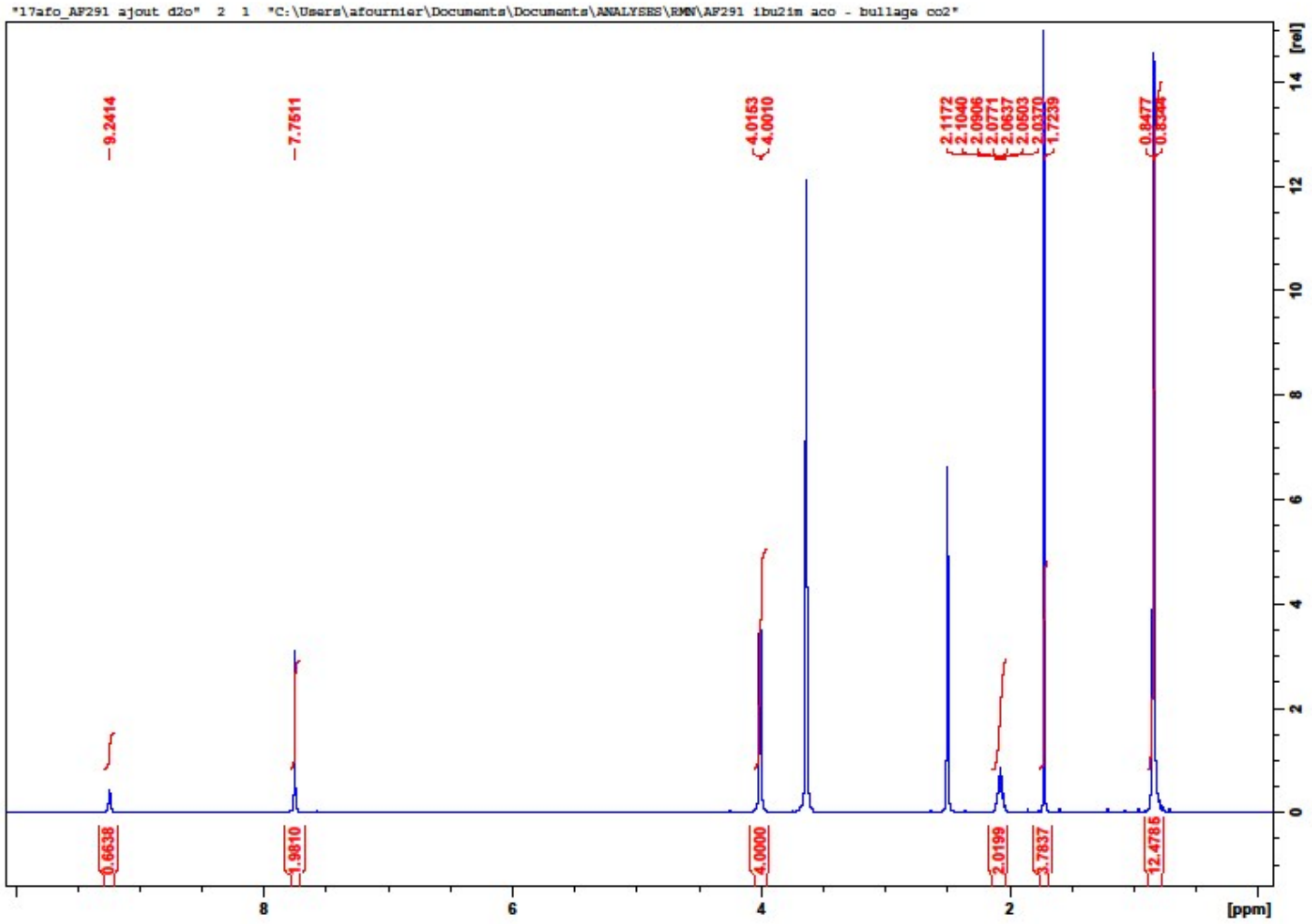
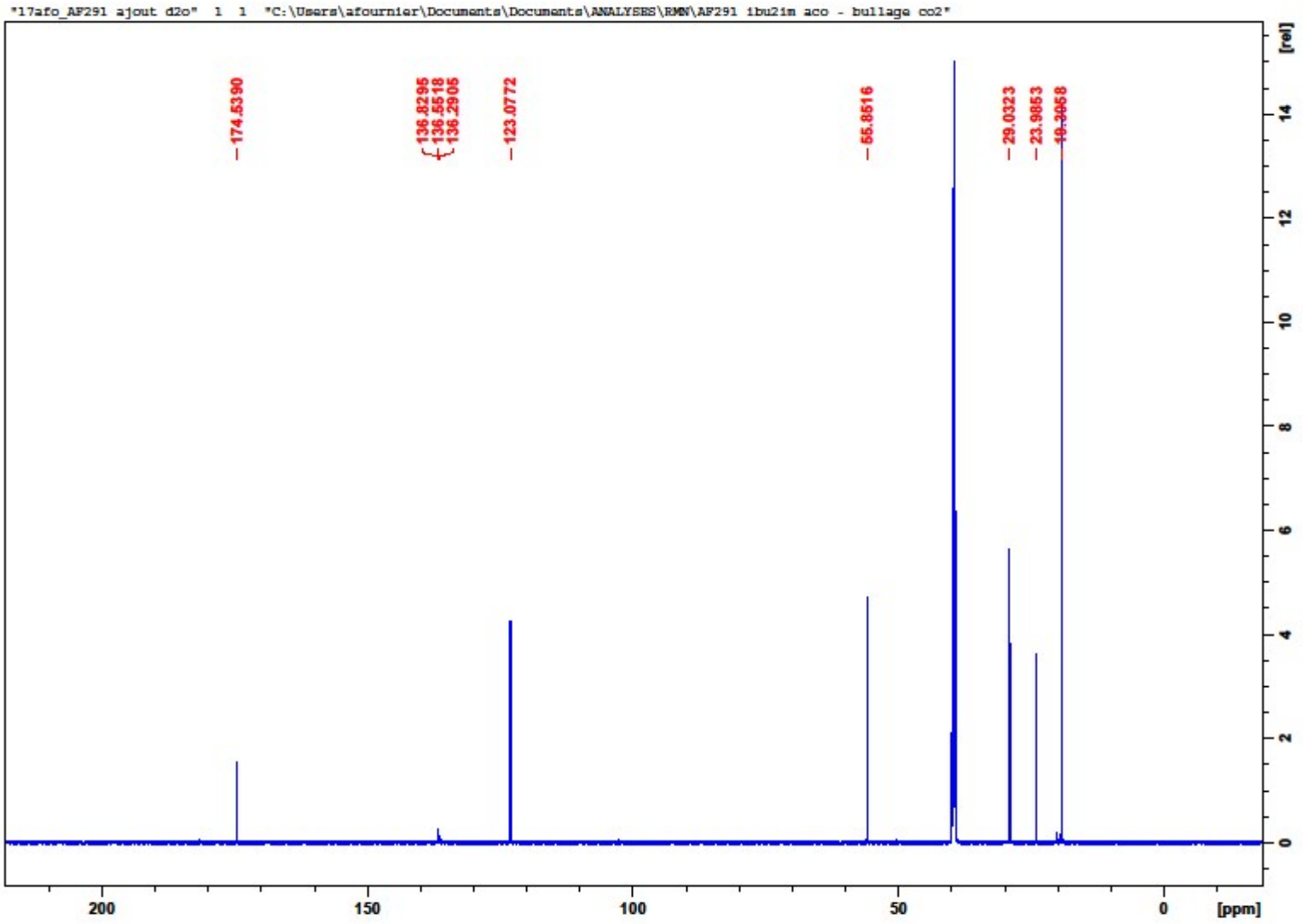
After addition of D_2O

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10
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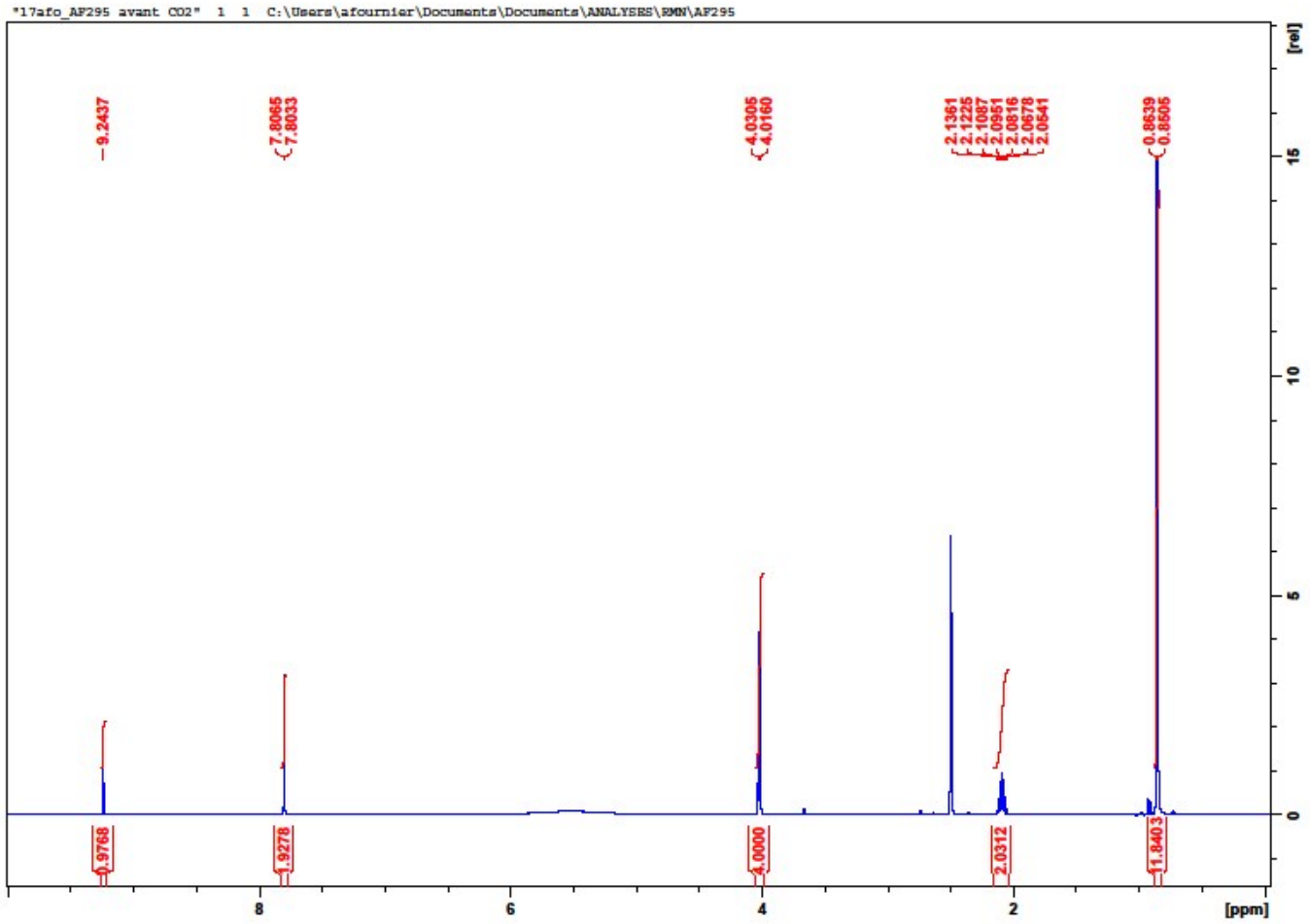
Experiments of CO_2 chemisorption with [*i*Bu_2IM](HC_2O_4):

Before CO_2 bubbling:



After CO_2 bubbling: