

碳谱中的溶剂峰

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做碳谱的时候, 如果氘代试剂不纯, 或者样品没有抽干 (含有其他溶剂), 碳谱就会含有其他溶剂的峰, 干扰对样品的分析。通过查下表, 我们可以排出这些干扰

Table 2. ^{13}C NMR Data^a

		CDCl_3	$(\text{CD}_3)_2\text{CO}$	$(\text{CD}_3)_2\text{SO}$	C_6D_6	CD_3CN	CD_3OD	D_2O
solvent signals		77.16 ± 0.06	29.84 ± 0.01 206.26 ± 0.13	39.52 ± 0.06	128.06 ± 0.02	1.32 ± 0.02 118.26 ± 0.02	49.00 ± 0.01	
acetic acid	CO	175.99	172.31	171.93	175.82	173.21	175.11	177.21
	CH ₃	20.81	20.51	20.95	20.37	20.73	20.56	21.03
acetone	CO	207.07	205.87	206.31	204.43	207.43	209.67	215.94
	CH ₃	30.92	30.60	30.56	30.14	30.91	30.67	30.89
acetonitrile	CN	116.43	117.60	117.91	116.02	118.26	118.06	119.68
	CH ₃	1.89	1.12	1.03	0.20	1.79	0.85	1.47
benzene	CH	128.37	129.15	128.30	128.62	129.32	129.34	
tert-butyl alcohol	C	69.15	68.13	66.88	68.19	68.74	69.40	70.36
	CH ₃	31.25	30.72	30.38	30.47	30.68	30.91	30.29
tert-butyl methyl ether	OCH ₃	49.45	49.35	48.70	49.19	49.52	49.66	49.37
	C	72.87	72.81	72.04	72.40	73.17	74.32	75.62
	CCH ₃	26.99	27.24	26.79	27.09	27.28	27.22	26.60
BHT	C(1)	151.55	152.51	151.47	152.05	152.42	152.85	
	C(2)	135.87	138.19	139.12	136.08	138.13	139.09	
	CH(3)	125.55	129.05	127.97	128.52	129.61	129.49	
	C(4)	128.27	126.03	124.85	125.83	126.38	126.11	
	CH ₃ Ar	21.20	21.31	20.97	21.40	21.23	21.38	
	CH ₃ C	30.33	31.61	31.25	31.34	31.50	31.15	
	C	34.25	35.00	34.33	34.35	35.05	35.36	
chloroform	CH	77.36	79.19	79.16	77.79	79.17	79.44	
cyclohexane	CH ₂	26.94	27.51	26.33	27.23	27.63	27.96	
1,2-dichloroethane	CH ₂	43.50	45.25	45.02	43.59	45.54	45.11	
dichloromethane	CH ₂	53.52	54.95	54.84	53.46	55.32	54.78	
diethyl ether	CH ₃	15.20	15.78	15.12	15.46	15.63	15.46	14.77
	CH ₂	65.91	66.12	62.05	65.94	66.32	66.88	66.42
diglyme	CH ₃	59.01	58.77	57.98	58.66	58.90	59.06	58.67
	CH ₂	70.51	71.03	69.54	70.87	70.99	71.33	70.05
	CH ₂	71.90	72.63	71.25	72.35	72.63	72.92	71.63
1,2-dimethoxyethane	CH ₃	59.08	58.45	58.01	58.68	58.89	59.06	58.67
	CH ₂	71.84	72.47	71.07	72.21	72.47	72.72	71.49
dimethylacetamide	CH ₃	21.53	21.51	21.29	21.16	21.76	21.32	21.09
	CO	171.07	170.61	169.54	169.95	171.31	173.32	174.57
	NCH ₃	35.28	34.89	37.38	34.67	35.17	35.50	35.03
	NCH ₃	38.13	37.92	34.42	37.03	38.26	38.43	38.76
dimethylformamide	CH	162.62	162.79	162.29	162.13	163.31	164.73	165.53
	CH ₃	36.50	36.15	35.73	35.25	36.57	36.89	37.54
	CH ₃	31.45	31.03	30.73	30.72	31.32	31.61	32.03
dimethyl sulfoxide	CH ₃	40.76	41.23	40.45	40.03	41.31	40.45	39.39
dioxane	CH ₂	67.14	67.60	66.36	67.16	67.72	68.11	67.19
ethanol	CH ₃	18.41	18.89	18.51	18.72	18.80	18.40	17.47
	CH ₂	58.28	57.72	56.07	57.86	57.96	58.26	58.05
ethyl acetate	CH ₃ CO	21.04	20.83	20.68	20.56	21.16	20.88	21.15
	CO	171.36	170.96	170.31	170.44	171.68	172.89	175.26
	CH ₂	60.49	60.56	59.74	60.21	60.98	61.50	62.32
	CH ₃	14.19	14.50	14.40	14.19	14.54	14.49	13.92
ethyl methyl ketone	CH ₃ CO	29.49	29.30	29.26	28.56	29.60	29.39	29.49
	CO	209.56	208.30	208.72	206.55	209.88	212.16	218.43
	CH ₂ CH ₃	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	CH ₂ CH ₃	7.86	8.03	7.61	7.91	8.14	8.09	7.87
ethylene glycol	CH ₂	63.79	64.26	62.76	64.34	64.22	64.30	63.17
	CH ₂	29.76	30.73	29.20	30.21	30.86	31.29	
"grease"	CH ₃	14.14	14.34	13.88	14.32	14.43	14.45	
<i>n</i> -hexane	CH ₂ (2)	22.70	23.28	22.05	23.04	23.40	23.68	
	CH ₂ (3)	31.64	32.30	30.95	31.96	32.36	32.73	
	CH ₃	36.87	37.04	36.42	36.88	37.10	37.00	36.46
HMPA ^b	CH ₃	50.41	49.77	48.59	49.97	49.90	49.86	49.50 ^c
methanol	CH ₃	62.50	63.21	63.28	61.16	63.66	63.08	63.22
nitromethane	CH ₃	14.08	14.29	13.28	14.25	14.37	14.39	
	CH ₂ (2)	22.38	22.98	21.70	22.72	23.08	23.38	
	CH ₂ (3)	34.16	34.83	33.48	34.45	34.89	35.30	
2-propanol	CH ₃	25.14	25.67	25.43	25.18	25.55	25.27	24.38
	CH	64.50	63.85	64.92	64.23	64.30	64.71	64.88
pyridine	CH(2)	149.90	150.67	149.58	150.27	150.76	150.07	149.18
	CH(3)	123.75	124.57	123.84	123.58	127.76	125.53	125.12
	CH(4)	135.96	136.56	136.05	135.28	136.89	138.35	138.27
silicone grease	CH ₃	1.04	1.40		1.38		2.10	
	CH ₂	25.62	26.15	25.14	25.72	26.27	26.48	25.67
tetrahydrofuran	CH ₂ O	67.97	68.07	67.03	67.80	68.33	68.83	68.68
	CH ₃	21.46	21.46	20.99	21.10	21.50	21.50	
toluene	C(<i>f</i>)	137.89	138.48	137.35	137.91	138.90	138.85	
	CH(<i>o</i>)	129.07	129.76	128.88	129.33	129.94	129.91	
	CH(<i>m</i>)	128.26	129.03	128.18	128.56	129.23	129.20	
	CH(<i>p</i>)	125.33	126.12	125.29	125.68	126.28	126.29	
triethylamine	CH ₃	11.61	12.49	11.74	12.35	12.38	11.09	9.07
	CH ₂	46.25	47.07	45.74	46.77	47.10	46.96	47.19

^a See footnotes for Table 1. ^b $J_{\text{FC}} = 3 \text{ Hz}$. ^c Reference material; see text.

比如: 有一个样品, 氘代试剂是氘代氯仿, 如果谱图在207, 31左右有两个峰无法归属, 通过查表 (第三行), 我们可以确定这是一个丙酮峰. 应该是样品中含有少量丙酮。