

碳谱化学位移表

常见杂质	carbon	THF-d8	CD ₂ Cl ₂	CDCl ₃	Toluene-d8	C ₆ D ₆	C ₆ D ₅ Cl	(CD ₃) ₂ CO	(CD ₃) ₂ S O	CD ₃ CN	TFE-d ₃	CD ₃ OD	D ₂ O
solvent signals		67.21/25.3 1	53.84	77.16	137.48/128.87 /127.96/125.13 /20.43	128.06	134.19/129.26 /128.25/125.96	29.84/206.26	39.52	1.32/118.2 6	61.5/126.28	49	-
acetic acid	CO	171.69	175.85	175.99	175.3	175.82	175.67	172.31	171.93	173.21	177.96	175.11	177.21
acetic acid	CH ₃	20.13	20.91	20.81	20.27	20.37	20.4	20.51	20.95	20.73	20.91	20.56	21.03
acetone	CO	204.19	206.78	207.07	204	204.43	204.83	205.87	206.31	207.43	32.35	209.67	215.94
acetone	CH ₃	30.17	31	30.92	30.03	30.14	30.12	30.6	30.56	30.91	214.98	30.67	30.89
acetonitrile	CN	116.79	116.92	116.43	115.76	116.02	115.93	117.6	117.91	118.26	118.95	118.06	119.68
acetonitrile	CH ₃	0.45	2.03	1.89	0.03	0.2	0.63	1.12	1.03	1.79	1	0.85	1.47
allyl acetate	CO	170.14	170.83	170.81	169.44	169.67	169.59	170.61	169.97	171.32	175.98	172.41	174.78
allyl acetate	CHCH ₂	133.9	132.94	132.33	132.98	132.9	132.69	133.76	132.71	133.83	133.33	133.71	132.48
allyl acetate	CHCH ₂	117.58	118	118.34	117.49	117.64	117.63	117.81	117.64	118.06	119.39	118.22	119.03
allyl acetate	CH ₂	65.31	65.36	65.28	64.87	64.92	64.86	65.28	64.32	65.55	67.61	66.14	66.52
allyl acetate	CH ₃	20.45	21.06	21.02	20.21	20.37	20.4	20.68	20.54	21.02	21.1	20.71	21
benzaldehyde	HCO	191.95	192.61	192.67	191.09	191.43	191.24	192.95	193.08	193.64	197.63	194.11	191.67
benzaldehyde	C(1)	137.78	136.98	136.58	137.12	137.05	136.78	137.66	136.2	137.62	137.84	137.96	136.11
benzaldehyde	CH(2,6)	129.98	129.98	129.91	129.61	129.65	129.49	130.23	129.45	130.42	131.78	130.64	130.09

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常见杂质	carbon	THF-d8	CD2Cl2	CDCl3	Toluene-d8	C6D6	C6D5Cl	(CD3)2CO	(CD3)2S O	CD3CN	TFE-d3	CD3OD	D2O
benzaldehyde	CH(3,5)	129.56	129.42	129.16	128.68	128.95	128.87	129.9	129.1	130.07	130.82	130.12	129.48
benzaldehyde	CH(4)	134.67	134.79	134.64	133.88	133.95	134.02	135.14	134.52	135.4	137.17	135.6	134.7
benzene	CH	128.84	128.68	128.37	128.57	128.62	128.38	129.15	128.3	129.32	129.84	129.34	-
tert-butyl alcohol	(CH3)3C	67.5	69.11	69.15	68.12	68.19	68.19	68.13	66.88	68.74	72.35	69.4	70.36
tert-butyl alcohol	(CH3)3C	30.57	31.46	31.25	30.49	30.47	31.13	30.72	30.38	30.68	31.07	30.91	30.29
BHA	C(1)	154.07	153.05	152.57	153.5	153.62	153.19	153.97	152.53	154.02	153.74	154.34	-
BHA	C(2,6)	148.62	148.06	147.85	148.06	148.13	147.87	148.48	147.44	148.39	150.52	149.04	-
BHA	CH(3,5)	110.94	110.93	110.69	110.99	111.15	110.84	111	109.8	111.35	112.9	111.3	-
BHA	C(4)	140.07	137.77	137.36	137.34	137.5	137.29	140.32	141.16	140.2	140.23	141.36	-
BHA	CH3O	55.39	55.88	55.7	55.04	55.27	55.08	55.51	54.89	55.94	57.55	55.96	-
BHA	(CH3)3C	30.65	30.37	30.32	30.3	30.35	30.21	30.64	30.3	30.55	30.8	30.82	-
BHA	(CH3)3C	35.51	34.91	34.72	34.69	34.72	34.56	35.45	34.76	35.48	36.07	35.83	-
BHT	C(1)	152.48	151.92	151.55	152.06	152.05	151.69	152.51	151.47	152.42	153.46	152.85	-
BHT	C(2,6)	137.93	136.32	135.87	136.12	136.08	135.92	138.19	139.12	138.13	138.59	139.09	-
BHT	CH(3,5)	125.71	125.84	125.55	125.79	125.83	125.58	126.03	124.85	126.38	127.11	126.11	-

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常见杂质	carbon	THF-d8	CD2Cl2	CDCl3	Toluene-d8	C6D6	C6D5Cl	(CD3)2CO	(CD3)2S O	CD3CN	TFE-d3	CD3OD	D2O
BHT	C(4)	128.64	128.73	128.27	128.44	128.52	128.26	129.05	127.97	129.61	130.62	129.49	-
BHT	CH3Ar	21.21	21.27	21.2	21.42	21.4	21.1	21.31	20.97	21.23	21.34	21.38	-
BHT	(CH3)3C	31.55	30.54	30.33	31.39	31.34	30.19	31.61	31.25	31.5	31.01	31.15	-
BHT	(CH3)3C	34.91	34.56	34.25	34.39	34.35	34.11	35	34.33	35.05	35.69	35.36	-
carbon dioxide	CO2	125.69	125.26	124.99	124.86	124.76	126.08	125.81	124.21	125.89	126.92	126.31	-
carbon disulfide	CS2	193.37	192.95	192.83	192.71	192.69	192.49	193.58	192.63	193.6	196.26	193.82	197.25
carbon tetrachloride	CCl4	96.89	96.52	96.34	96.57	96.44	96.38	96.65	95.44	96.68	97.74	97.21	96.73
chloroform	CH	79.24	77.99	77.36	77.89	77.79	77.67	79.19	79.16	79.17	78.83	79.44	-
18-crown-6	CH2	71.34	70.47	70.55	70.86	70.59	70.55	71.25	69.85	71.22	70.8	71.47	70.14
cyclohexane	CH2	27.58	27.38	26.94	27.31	27.23	26.99	27.51	26.33	27.63	28.34	27.96	-
cyclohexanone	CO	208.79	211.82	212.57	208.6	209.1	209.3	210.36	210.63	211.99	221.3	214.69	221.22
cyclohexanone	CH2(2,6)	42.17	42.31	41.97	41.78	41.83	41.79	42.24	41.32	42.44	43.16	42.61	42.02
cyclohexanone	CH2(3,5)	27.69	27.47	27	27.05	27	27.02	27.68	26.46	27.8	28.56	28.16	27.5
cyclohexanone	CH2(4)	25.76	25.42	24.97	25.15	25.03	25.07	25.59	24.32	25.62	26	25.86	24.77
diallyl carbonate	CO	155.36	155.15	154.88	155.15	155.24	154.87	155.48	154.16	155.66	157.39	156.28	157.78

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常见杂质	carbon	THF-d8	CD2Cl2	CDCl3	Toluene-d8	C6D6	C6D5Cl	(CD3)2CO	(CD3)2S O	CD3CN	TFE-d3	CD3OD	D2O
diallyl carbonate	CHCH2	133.08	132.24	131.58	132.3	132.18	131.93	133.16	132.18	133.2	132.72	133.25	132.76
diallyl carbonate	CHCH2	117.7	118.75	118.96	118.04	118.22	118.22	118.53	118.32	118.86	120.15	118.74	118.75
diallyl carbonate	CH2	68.58	68.76	68.55	68.2	68.28	68.19	68.78	67.86	69.09	70.69	69.35	68.81
1,2-dichloroethane	CH2	44.64	44.35	43.5	43.4	43.59	43.6	45.25	45.02	45.54	45.28	45.11	-
dichloromethane	CH2	54.67	54.24	53.52	53.47	53.46	53.54	54.95	54.84	55.32	54.46	54.78	-
diethyl ether	CH3	15.49	15.44	15.2	15.47	15.46	15.35	15.78	15.12	15.63	15.33	15.46	14.77
diethyl ether	CH2	66.14	66.11	65.91	65.94	65.94	65.79	66.12	62.05	66.32	67.55	66.88	66.42
diglyme	CH3	58.72	58.95	59.01	58.62	58.66	58.42	58.77	57.98	58.9	59.4	59.06	58.67
diglyme	CH2	71.17	70.7	70.51	70.92	70.87	70.56	71.03	69.54	70.99	73.05	71.33	70.05
diglyme	CH2	72.72	72.25	71.9	72.39	72.35	72.07	72.63	71.25	72.63	71.33	72.92	71.63
1,2-dimethoxyethane	CH3	58.72	59.02	59.08	58.63	58.68	58.31	58.45	58.03	58.89	59.52	59.06	58.67
1,2-dimethoxyethane	CH2	72.58	72.24	71.84	72.25	72.21	71.81	72.47	71.17	72.47	72.87	72.72	71.49
dimethylacetamide	CH3	21.15	21.64	21.53	21.05	21.16	21.03	21.51	21.29	21.76	21.4	21.32	21.09
dimethylacetamide	CO	169.77	171.05	171.07	169.65	169.95	169.79	170.61	169.54	171.31	175.74	173.32	174.57
dimethylacetamide	NCH3	34.6	35.23	35.28	34.58	34.67	34.59	34.89	34.42	35.17	36.28	35.5	35.03

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常见杂质	carbon	THF-d8	CD2Cl2	CDCl3	Toluene-d8	C6D6	C6D5Cl	(CD3)2CO	(CD3)2S O	CD3CN	TFE-d3	CD3OD	D2O
dimethylacetamide	NCH3	37.56	38.22	38.13	36.98	37.03	37.13	37.92	37.38	38.26	39.06	38.43	38.76
dimethyl carbonate	CO	156.91	156.73	156.45	156.61	156.71	156.36	157.04	155.76	157.26	159.04	157.91	163.96
dimethyl carbonate	CH3	54.58	55.09	54.89	54.13	54.3	54.23	54.95	54.63	55.39	56.17	55.25	55.81
dimethyl malonate	CO2	167.14	167.32	167.18	166.49	166.66	166.51	167.58	166.91	168.07	170.88	168.7	170.12
dimethyl malonate	CH3	52.07	52.75	52.57	51.76	51.86	51.89	52.47	52.08	52.95	54	52.83	53.65
dimethyl malonate	CH2	41.15	41.48	41.11	40.88	41.04	40.93	41.43	40.72	41.77	42.13	41.6	42.13
dimethylformamide	CH	161.96	162.57	162.62	161.93	162.13	162.01	162.79	162.29	163.31	166.01	164.73	165.53
dimethylformamide	CH3	35.65	36.56	36.5	35.22	35.25	35.45	36.15	35.73	36.57	37.76	36.89	37.54
dimethylformamide	CH3	30.7	31.39	31.45	30.64	30.72	30.71	31.03	30.73	31.32	30.96	31.61	32.03
dimethyl sulfoxide	CH3	41.21	41.33	40.76	40.41	40.03	40.27	41.23	40.45	41.31	40.06	40.45	39.39
1,4-dioxane	CH2	67.65	67.47	67.14	67.17	67.16	66.95	67.6	66.36	67.72	68.52	68.11	67.19
ethane	CH3	6.79	6.91	6.89	6.94	6.96	6.91	6.88	6.61	6.99	7.01	6.98	-
ethanol	CH3	18.9	18.69	18.41	18.78	18.72	18.55	18.89	18.51	18.8	18.11	18.4	17.47
ethanol	CH2	57.6	58.57	58.28	57.81	57.86	57.63	57.72	56.07	57.96	59.68	58.26	58.05
ethyl acetate	CH3CO	20.45	21.15	21.04	20.46	20.56	20.5	20.83	20.68	21.16	21.18	20.88	21.15

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常见杂质	carbon	THF-d8	CD2Cl2	CDCl3	Toluene-d8	C6D6	C6D5Cl	(CD3)2CO	(CD3)2S O	CD3CN	TFE-d3	CD3OD	D2O
ethyl acetate	CO	170.32	171.24	171.36	170.02	170.44	170.2	170.96	170.31	171.68	175.55	172.89	175.26
ethyl acetate	CH2	60.3	60.63	60.49	60.08	60.21	60.06	60.56	59.74	60.98	62.7	61.5	62.32
ethyl acetate	CH3	14.37	14.37	14.19	14.23	14.19	14.07	14.5	14.4	14.54	14.36	14.49	13.92
ethyl acetate ketone	CH3CO	28.92	29.55	29.49	28.74	28.56	28.82	29.3	29.26	29.6	29.64	29.39	29.49
ethyl acetate ketone	CO	207.05	209.57	209.56	206.31	206.55	206.87	208.3	208.72	209.88	218.31	212.16	218.43
ethyl acetate ketone	CH2CH3	36.59	37.01	36.89	36.32	36.36	36.39	36.75	35.83	37.09	38.23	37.34	37.27
ethyl acetate ketone	CH2CH3	7.87	7.94	7.86	7.89	7.91	7.79	8.03	7.61	8.14	8.29	8.09	7.87
ethylene	CH2	123.09	123.2	123.13	122.92	122.96	122.95	123.47	123.52	123.69	124.08	123.46	-
ethylene glycol	CH2	64.35	64.08	63.79	64.29	64.34	64.03	64.26	62.76	64.22	64.87	64.3	63.17
furan	CH(2,5)	143.26	142.98	142.71	142.65	142.73	142.49	143.49	142.82	143.74	144.22	143.68	143.57
furan	CH(3,4)	109.88	109.86	109.57	109.63	109.67	109.64	110.24	109.62	110.49	111.06	110.33	110.23
H grease8	CH2	30.45	30.14	29.71	30.31	30.22	30.11	-	-	-	-	-	-
hexamethylbenzene	C	131.88	132.09	132.21	131.72	131.79	131.54	132.22	131.1	132.61	134.04	132.53	-
hexamethylbenzene	CH3	16.71	16.93	16.98	16.84	16.95	16.68	16.86	16.6	16.94	17.04	16.9	-
hexamethyldisiloxane	CH3	1.83	1.96	1.97	1.99	2.05	1.92	2.01	1.96	2.07	2.09	1.99	2.31

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常见杂质	carbon	THF-d8	CD2Cl2	CDCl3	Toluene-d8	C6D6	C6D5Cl	(CD3)2CO	(CD3)2S O	CD3CN	TFE-d3	CD3OD	D2O
n-hexane	CH3	14.22	14.28	14.14	14.34	14.32	14.18	14.34	13.88	14.43	14.63	14.45	-
n-hexane	CH2(2,5)	23.33	23.07	22.7	23.12	23.04	22.86	23.28	22.05	23.4	24.06	23.68	-
n-hexane	CH2(3,4)	32.34	32.01	31.64	32.06	31.96	31.77	32.3	30.95	32.36	33.17	32.73	-
HMPA11	CH3	36.89	36.99	36.87	36.8	36.88	36.64	37.04	36.42	37.1	37.21	37	36.46
imidazole	CH(2)	135.72	135.76	135.38	135.57	135.76	135.5	135.89	135.15	136.33	136.58	136.31	136.65
imidazole	CH(4,5)	122.2	122.16	122	122.13	122.16	121.96	122.31	121.55	122.78	122.93	122.6	122.43
methane	CH4	-4.90	-4.33	-4.63	-4.34	-4.29	-4.33	-5.33	-4.01	-4.61	-5.88	-4.90	-
methanol	CH3	49.64	50.45	50.41	49.9	49.97	49.66	49.77	48.59	49.9	50.67	49.86	49.5012
nitromethane	CH3	62.49	63.03	62.5	61.14	61.16	61.68	63.21	63.28	63.66	63.17	63.08	63.22
n-pentane	CH3	14.18	14.24	14.08	14.27	14.25	14.1	14.29	13.28	14.37	14.54	14.39	-
n-pentane	CH2(2,4)	23	22.77	22.38	22.79	22.72	22.54	22.98	21.7	23.08	23.75	23.38	-
n-pentane	CH2(3)	34.87	34.57	34.16	34.54	34.45	34.26	34.83	33.48	34.89	35.76	35.3	-
propane	CH3	16.6	16.63	16.63	16.65	16.66	16.56	16.68	16.34	16.73	16.93	16.8	-
propane	CH2	16.82	16.63	16.37	16.63	16.6	16.48	16.78	15.67	16.91	17.46	17.19	-
2-propanol	CH3	25.7	25.43	25.14	25.24	25.18	25.14	25.67	25.43	25.55	25.21	25.27	24.38

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2-propanol	CH	66.14	64.67	64.5	64.12	64.23	64.18	63.85	64.92	64.3	66.69	64.71	64.88
propylene	CH3	19.27	19.47	19.5	19.32	19.38	19.32	19.42	19.2	19.48	19.63	19.5	-
propylene	CH2	115.74	115.7	115.74	115.89	115.92	115.86	116.03	116.07	116.12	116.38	116.04	-
propylene	CH	134.02	134.21	133.91	133.61	133.69	133.57	134.34	133.55	134.78	136	134.61	-
pump oil	CH2	30.63	30.13	29.84	30.33	30.24	30.11	30.36	29.33	30.86	31.85	31.35	-
pyridine	CH(2,6)	150.57	150.27	149.9	150.25	150.27	149.93	150.67	149.58	150.76	149.76	150.07	149.18
pyridine	CH(3,5)	124.08	124.06	123.75	123.46	123.58	123.49	124.57	123.84	127.76	126.27	125.53	125.12
pyridine	CH(4)	135.99	136.16	135.96	135.17	135.28	135.32	136.56	136.05	136.89	139.62	138.35	138.27
pyrrole	CH(2,5)	118.03	117.93	117.77	117.61	117.78	117.65	117.98	117.32	118.47	119.61	118.28	119.06
pyrrole	CH(3,4)	107.74	108.02	107.98	108.15	108.21	108.03	108.04	107.07	108.31	108.85	108.11	107.83
pyrrolidine10	CH2(2,5)	45.82	47.02	46.93	47.12	46.86	46.75	-	46.51	47.57	47.43	47.23	46.83
pyrrolidine10	CH2(3,4)	26.17	25.83	25.56	25.75	25.65	25.59	-	25.26	26.34	25.73	26.29	25.86
silicone grease	CH3	1.2	1.22	1.19	1.37	1.38	1.09	1.4	-	-	2.87	2.1	-
tetrahydrofuran	CH2(2,5)	68.03	68.16	67.97	67.75	67.8	67.64	68.07	67.03	68.33	69.53	68.83	68.68
tetrahydrofuran	CH2(3,4)	26.19	25.98	25.62	25.79	25.72	25.68	26.15	25.14	26.27	26.69	26.48	25.67

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常见杂质	carbon	THF-d8	CD ₂ Cl ₂	CDCl ₃	Toluene-d ₈	C ₆ D ₆	C ₆ D ₅ Cl	(CD ₃) ₂ CO	(CD ₃) ₂ S O	CD ₃ CN	TFE-d ₃	CD ₃ OD	D ₂ O
toluene	CH ₃	21.29	21.53	21.46	21.37	21.1	21.23	21.46	20.99	21.5	21.62	21.5	-
toluene	C(1)	138.24	138.36	137.89	137.84	137.91	137.65	138.48	137.35	138.9	139.92	138.85	-
toluene	CH(2,6)	129.47	129.35	129.07	129.33	129.33	129.12	129.76	128.88	129.94	130.58	129.91	-
toluene	CH(3,5)	128.71	128.54	128.26	128.51	128.56	128.31	129.03	128.18	129.23	129.79	129.2	-
toluene	CH(4)	125.84	125.62	125.33	125.66	125.68	125.43	126.12	125.29	126.28	126.82	126.29	-
triethylamine	CH ₃	12.51	12.12	11.61	12.39	12.35	11.87	12.49	11.74	12.38	9.51	11.09	9.07
triethylamine	CH ₂	47.18	46.75	46.25	46.82	46.77	46.36	47.07	45.74	47.1	48.45	46.96	47.19