

# NMR溶媒物理定数

## Constants of Deuterated NMR Solvents

Compound(Mol. Wt.)	$d_4^{20}$	m.p.	b.p.	$\sigma_H(\text{mult})$	$J_{HD}$	$\sigma_C(\text{mult})$	$J_{CD}(J_{CF})$
Acetic Acid-d <sub>4</sub> (64.078)	1.12	17	118	11.53(1) 2.03(5)	2	178.4(br) 20.0(7)	20
Acetone-d <sub>6</sub> (64.117)	0.87	-94	57	2.04(5)	2.2	206.0(13) 29.8(7)	0.9 20
Acetonitrile-d <sub>3</sub> (44.071)	0.84	-45	82	1.93(5)	2.5	118.2(br) 1.3(7)	21
Benzene-d <sub>6</sub> (84.152)	0.95	5	80	7.15(br)		128.0(3)	24
Chloroform-d <sub>1</sub> (120.384)	1.50	-64	62	7.24(1)		77.0(3)	32
Cyclohexane-d <sub>12</sub> (96.236)	0.89	6	81	1.38(br)		26.4(5)	19
Deuterium Oxide(20.028)	1.11	3.8	101.4	4.63(DSS) 4.67(TSP)			
1,2-Dichloroethane-d <sub>4</sub> (102.985)	1.25	-40	84	3.72(br)		43.6(5)	23.5
Diethyl-d <sub>10</sub> Ether(84.185)	0.82	-116	35	3.34(m) 1.07(m)		65.3(5) 14.5(7)	21 19
Dimethylformamide-d <sub>7</sub> (80.138)	1.04	-61	153	8.01(br) 2.91(5) 2.74(5)	2 2	162.7(3) 35.2(7) 30.1(7)	30 21 21
Dimethyl-d <sub>6</sub> Sulfoxide(84.170)	1.18	18	189	2.49(5)	1.7	39.5(7)	21
Ethyl Alcohol-d <sub>6</sub> (anh)(52.106)	0.91	≤ 130	79	5.19(1) 3.55(br) 1.11(m)		56.8(5) 17.2(7)	22 19
Hexafluoroacetone Deuterate(198.067)	1.71	21		5.26(1)		122.5(4) 92.9(7)	(287) (34.5)
Methyl Alcohol-d <sub>4</sub> (36.067)	0.89	-98	65	4.78(1) 3.30(5)	1.7	49.0(7)	21.5
Methyl Chloride-d <sub>2</sub> (86.945)	1.35	-95	40	5.32(3)	1	53.8(5)	27
Nitrobenzene-d <sub>5</sub> (128.143)	1.25	6	211	8.11(br) 7.67(br) 7.50(br)		148.6(1) 134.8(3) 129.5(3) 123.5(3)	24.5(p) 25 26
Nitromethane-d <sub>3</sub> (64.059)	1.20	-29	101	4.33(5)	2	62.8(7)	22
Pyridine-d <sub>5</sub> (84.133)	1.05	-42	116	8.71(br) 7.55(br) 7.19(br)		149.9(3) 135.5(3) 123.5(3)	27.5 24.5(g) 25
Tetrahydrofuran-d <sub>8</sub> (80.157)	0.99	-109	66	3.58(br) 1.73(br)		67.4(5) 25.3(br)	22 20.5
Toluene-d <sub>8</sub> (100.91)	0.94	-95	111	7.09(m) 7.00(br) 6.98(m) 2.09(5)	2.3	137.5(1) 128.9(3) 128.0(3) 125.2(3) 20.4(7)	23 24 24(p) 19
Trifluoroacetic Acide-d <sub>1</sub> (115.030)	1.50	-15	72	11.50(1)		164.2(4) 116.6(4)	(44) (283)
2,2,2-Trifluoroethyl Alcohol-d <sub>3</sub> (103.059)	1.45	-44	75	5.02(1) 3.88(4×3)	2(9)	126.3(4) 61.5(4×5)	(277) 22(36)