

EXACT MASS

	Dalton (a.m.u.)
proton	1.00728
neutron	1.00866
electron	0.0005486

List of possible molecular formulas by exact mass

Allowed molecular formula: C₃₋₁₀H₀₋₂₀N₀₋₂O₀₋₃Cl₀₋₁

Mass range : 100-200

Insaturation: 0-7 (must be an integer)

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C ₅ H ₅ Cl	100,00798	C ₅ H ₁₁ Cl	106,05493	C ₅ H ₆ O ₃	114,03170	C ₃ HClO ₃	119,96142
C ₄ H ₄ O ₃	100,01604	C ₄ H ₁₀ O ₃	106,06300	C ₄ H ₆ N ₂ O ₂	114,04293	C ₇ HCl	119,97668
C ₃ H ₄ N ₂ O ₂	100,02728	C ₃ H ₁₀ N ₂ O ₂	106,07423	C ₉ H ₆	114,04695	C ₆ O ₃	119,98474
C ₈ H ₄	100,03130	C ₈ H ₁₀	106,07825	C ₆ H ₁₀ O ₂	114,06808	C ₅ N ₂ O ₂	119,99598
C ₅ H ₈ O ₂	100,05243	C ₅ HNO ₂	107,00073	C ₅ H ₁₀ N ₂ O	114,07931	C ₄ H ₅ ClO ₂	119,99781
C ₄ H ₈ N ₂ O	100,06366	C ₃ H ₆ CINO	107,01379	C ₇ H ₁₄ O	114,10446	C ₃ H ₅ CIN ₂ O	120,00904
C ₆ H ₁₂ O	100,08882	C ₆ H ₅ NO	107,03711	C ₆ H ₁₄ N ₂	114,11570	C ₇ H ₄ O ₂	120,02113
C ₅ H ₁₂ N ₂	100,10005	C ₄ H ₁₀ CIN	107,05018	C ₈ H ₁₈	114,14085	C ₆ H ₄ N ₂ O	120,03236
C ₇ H ₁₆	100,12520	C ₃ H ₉ NO ₃	107,05824	C ₄ H ₂ CINO	114,98249	C ₅ H ₉ ClO	120,03419
C ₃ CINO	100,96684	C ₇ H ₉ N	107,07350	C ₅ H ₆ CIN	115,01888	C ₄ H ₃ CIN ₂	120,04543
C ₄ H ₄ CIN	101,00323	C ₆ HCl	107,97668	C ₄ H ₅ NO ₃	115,02694	C ₃ H ₈ N ₂ O ₃	120,05349
C ₃ H ₃ NO ₃	101,01129	C ₅ O ₃	107,98474	C ₈ H ₅ N	115,04220	C ₈ H ₈ O	120,05752
C ₇ H ₃ N	101,02655	C ₄ N ₂ O ₂	107,99598	C ₅ H ₉ NO ₂	115,06333	C ₇ H ₈ N ₂	120,06875
C ₄ H ₇ NO ₂	101,04768	C ₃ H ₅ ClO ₂	107,99781	C ₆ H ₁₃ NO	115,09971	C ₆ H ₁₃ Cl	120,07058
C ₅ H ₁₁ NO	101,08406	C ₆ H ₄ O ₂	108,02113	C ₇ H ₁₇ N	115,13610	C ₅ H ₁₂ O ₃	120,07865
C ₆ H ₁₅ N	101,12045	C ₃ H ₄ N ₂ O	108,03236	C ₄ HClO ₂	115,96651	C ₄ H ₁₂ N ₂ O ₂	120,08988
C ₄ H ₃ ClO	101,98724	C ₄ H ₉ ClO	108,03419	C ₃ HCIN ₂ O	115,97774	C ₉ H ₁₂	120,09390
C ₃ H ₃ CIN ₂	101,99848	C ₃ H ₉ CIN ₂	108,04543	C ₅ H ₅ ClO	116,00289	C ₆ CIN	120,97193
C ₇ H ₂ O	102,01056	C ₇ H ₈ O	108,05752	C ₄ H ₅ CIN ₂	116,01413	C ₃ H ₄ CINO ₂	120,99306
C ₆ H ₂ N ₂	102,02180	C ₆ H ₈ N ₂	108,06875	C ₃ H ₄ N ₂ O ₃	116,02219	C ₆ H ₃ NO ₂	121,01638
C ₅ H ₇ Cl	102,02363	C ₈ H ₁₂	108,09390	C ₈ H ₄ O	116,02622	C ₄ H ₆ CINO	121,02944
C ₄ H ₆ O ₃	102,03170	C ₅ CIN	108,97193	C ₇ H ₄ N ₂	116,03745	C ₇ H ₇ NO	121,05276
C ₃ H ₆ N ₂ O ₂	102,04293	C ₅ H ₃ NO ₂	109,01638	C ₆ H ₉ Cl	116,03928	C ₅ H ₁₂ CIN	121,06583
C ₈ H ₆	102,04695	C ₃ H ₈ CINO	109,02944	C ₅ H ₈ O ₃	116,04734	C ₄ H ₁₁ NO ₃	121,07389
C ₅ H ₁₀ O ₂	102,06808	C ₆ H ₇ NO	109,05276	C ₄ H ₈ N ₂ O ₂	116,05858	C ₈ H ₁₁ N	121,08915
C ₄ H ₁₀ N ₂ O	102,07931	C ₇ H ₁₁ N	109,08915	C ₉ H ₈	116,06260	C ₃ H ₃ ClO ₃	121,97707
C ₆ H ₁₄ O	102,10446	C ₆ H ₃ Cl	109,99233	C ₆ H ₁₂ O ₂	116,08373	C ₇ H ₃ Cl	121,99233
C ₅ H ₁₄ N ₂	102,11570	C ₅ H ₂ O ₃	110,00040	C ₅ H ₁₂ N ₂ O	116,09496	C ₆ H ₂ O ₃	122,00040
C ₃ H ₂ CINO	102,98249	C ₄ H ₂ N ₂ O ₂	110,01163	C ₇ H ₁₆ O	116,12012	C ₅ H ₂ N ₂ O ₂	122,01163
C ₆ HNO	103,00581	C ₃ H ₇ ClO ₂	110,01346	C ₆ H ₁₆ N ₂	116,13135	C ₄ H ₇ ClO ₂	122,01346
C ₄ H ₆ CIN	103,01888	C ₆ H ₆ O ₂	110,03678	C ₃ CINO ₂	116,96176	C ₃ H ₇ CIN ₂ O	122,02469
C ₃ H ₅ NO ₃	103,02694	C ₅ H ₆ N ₂ O	110,04801	C ₄ H ₄ CINO	116,99814	C ₇ H ₆ O ₂	122,03678
C ₇ H ₅ N	103,04220	C ₇ H ₁₀ O	110,07316	C ₇ H ₃ NO	117,02146	C ₆ H ₆ N ₂ O	122,04801
C ₄ H ₉ NO ₂	103,06333	C ₆ H ₁₀ N ₂	110,08440	C ₅ H ₈ CIN	117,03453	C ₅ H ₁₁ ClO	122,04984
C ₅ H ₁₃ NO	103,09971	C ₈ H ₁₄	110,10955	C ₄ H ₇ NO ₃	117,04259	C ₄ H ₁₁ CIN ₂	122,06108
C ₃ HClO ₂	103,96651	C ₅ H ₂ CIN	110,98758	C ₈ H ₇ N	117,05785	C ₃ H ₁₀ N ₂ O ₃	122,06914
C ₆ O ₂	103,98983	C ₄ HNO ₃	110,99564	C ₅ H ₁₁ NO ₂	117,07898	C ₈ H ₁₀ O	122,07316
C ₅ N ₂ O	104,00106	C ₅ H ₅ NO ₂	111,03203	C ₆ H ₁₅ NO	117,11536	C ₇ H ₁₀ N ₂	122,08440
C ₄ H ₅ ClO	104,00289	C ₆ H ₉ NO	111,06841	C ₄ H ₃ ClO ₂	117,98216	C ₉ H ₁₄	122,10955
C ₃ H ₅ CIN ₂	104,01413	C ₇ H ₁₃ N	111,10480	C ₃ H ₃ CIN ₂ O	117,99339	C ₆ H ₂ CIN	122,98758
C ₇ H ₄ O	104,02622	C ₅ HClO	111,97159	C ₇ H ₂ O ₂	118,00548	C ₅ HNO ₃	122,99564
C ₆ H ₄ N ₂	104,03745	C ₄ HCIN ₂	111,98283	C ₆ H ₂ N ₂ O	118,01671	C ₃ H ₆ CINO ₂	123,00871
C ₅ H ₉ Cl	104,03928	C ₃ N ₂ O ₃	111,99089	C ₅ H ₇ ClO	118,01854	C ₆ H ₅ NO ₂	123,03203
C ₄ H ₈ O ₃	104,04734	C ₆ H ₅ Cl	112,00798	C ₄ H ₇ CIN ₂	118,02978	C ₄ H ₁₀ CINO	123,04509
C ₃ H ₈ N ₂ O ₂	104,05858	C ₅ H ₄ O ₃	112,01604	C ₃ H ₆ N ₂ O ₃	118,03784	C ₇ H ₉ NO	123,06841
C ₈ H ₈	104,06260	C ₄ H ₄ N ₂ O ₂	112,02728	C ₈ H ₆ O	118,04186	C ₈ H ₁₃ N	123,10480
C ₅ H ₁₂ O ₂	104,08373	C ₆ H ₈ O ₂	112,05243	C ₇ H ₆ N ₂	118,05310	C ₆ HClO	123,97159
C ₄ H ₁₂ N ₂ O	104,09496	C ₅ H ₈ N ₂ O	112,06366	C ₆ H ₁₁ Cl	118,05493	C ₅ HCIN ₂	123,98283
C ₃ H ₄ CINO	104,99814	C ₇ H ₁₂ O	112,08882	C ₅ H ₁₀ O ₃	118,06300	C ₄ N ₂ O ₃	123,99089
C ₆ H ₃ NO	105,02146	C ₆ H ₁₂ N ₂	112,10005	C ₄ H ₁₀ N ₂ O ₂	118,07423	C ₃ H ₅ ClO ₃	123,99272
C ₄ H ₈ CIN	105,03453	C ₈ H ₁₆	112,12520	C ₉ H ₁₀	118,07825	C ₇ H ₅ Cl	124,00798
C ₃ H ₇ NO ₃	105,04259	C ₄ CINO	112,96684	C ₆ H ₁₄ O ₂	118,09938	C ₆ H ₄ O ₃	124,01604
C ₇ H ₇ N	105,05785	C ₅ H ₄ CIN	113,00323	C ₅ H ₁₄ N ₂ O	118,11061	C ₅ H ₄ N ₂ O ₂	124,02728
C ₄ H ₁₁ NO ₂	105,07898	C ₄ H ₃ NO ₃	113,01129	C ₃ H ₂ CINO ₂	118,97741	C ₄ H ₉ ClO ₂	124,02911
C ₃ H ₃ ClO ₂	105,98216	C ₅ H ₇ NO ₂	113,04768	C ₆ HNO ₂	119,00073	C ₃ H ₉ CIN ₂ O	124,04034
C ₆ H ₂ O ₂	106,00548	C ₆ H ₁₁ NO	113,08406	C ₄ H ₆ CINO	119,01379	C ₇ H ₈ O ₂	124,05243
C ₅ H ₂ N ₂ O	106,01671	C ₇ H ₁₅ N	113,12045	C ₇ H ₅ NO	119,03711	C ₆ H ₈ N ₂ O	124,06366
C ₄ H ₇ ClO	106,01854	C ₅ H ₃ ClO	113,98724	C ₅ H ₁₀ CIN	119,05018	C ₈ H ₁₂ O	124,08882
C ₃ H ₇ CIN ₂	106,02978	C ₄ H ₃ CIN ₂	113,99848	C ₄ H ₉ NO ₃	119,05824	C ₇ H ₁₂ N ₂	124,10005
C ₇ H ₆ O	106,04186	C ₃ H ₂ N ₂ O ₃	114,00654	C ₈ H ₉ N	119,07350	C ₉ H ₁₆	124,12520
C ₆ H ₆ N ₂	106,05310	C ₆ H ₇ Cl	114,02363	C ₅ H ₁₃ NO ₂	119,09463	C ₅ CINO	124,96684

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C ₆ H ₄ CIN	125,00323	C ₇ H ₁₇ NO	131,13101	C ₅ H ₁₃ CIN ₂	136,07673	C ₈ H ₁₄ O ₂	142,09938
C ₅ H ₃ NO ₃	125,01129	C ₄ HClO ₃	131,96142	C ₄ H ₁₂ N ₂ O ₃	136,08479	C ₇ H ₁₄ N ₂ O	142,11061
C ₃ H ₈ CINO ₂	125,02436	C ₃ HCIN ₂ O ₂	131,97266	C ₉ H ₁₂ O	136,08882	C ₉ H ₁₈ O	142,13576
C ₆ H ₇ NO ₂	125,04768	C ₅ H ₅ ClO ₂	131,99781	C ₈ H ₁₂ N ₂	136,10005	C ₈ H ₁₈ N ₂	142,14700
C ₇ H ₁₁ NO	125,08406	C ₄ H ₅ CIN ₂ O	132,00904	C ₁₀ H ₁₆	136,12520	C ₅ H ₂ CINO ₂	142,97741
C ₈ H ₁₅ N	125,12045	C ₈ H ₄ O ₂	132,02113	C ₆ CINO	136,96684	C ₆ H ₆ CINO	143,01379
C ₆ H ₃ ClO	125,98724	C ₇ H ₄ N ₂ O	132,03236	C ₃ H ₄ CINO ₃	136,98797	C ₇ H ₁₀ CIN	143,05018
C ₅ H ₃ CIN ₂	125,99848	C ₆ H ₉ ClO	132,03419	C ₇ H ₄ CIN	137,00323	C ₆ H ₉ NO ₃	143,05824
C ₄ H ₂ N ₂ O ₃	126,00654	C ₅ H ₉ CIN ₂	132,04543	C ₈ H ₃ NO ₃	137,01129	C ₁₀ H ₉ N	143,07350
C ₃ H ₇ ClO ₃	126,00837	C ₄ H ₈ N ₂ O ₃	132,05349	C ₄ H ₈ CINO ₂	137,02436	C ₇ H ₁₃ NO ₂	143,09463
C ₇ H ₇ Cl	126,02363	C ₉ H ₈ O	132,05752	C ₇ H ₇ NO ₂	137,04768	C ₈ H ₁₇ NO	143,13101
C ₆ H ₆ O ₃	126,03170	C ₈ H ₈ N ₂	132,06875	C ₅ H ₁₂ CINO	137,06074	C ₅ HClO ₃	143,96142
C ₅ H ₆ N ₂ O ₂	126,04293	C ₇ H ₁₃ Cl	132,07058	C ₈ H ₁₁ NO	137,08406	C ₄ HCIN ₂ O ₂	143,97266
C ₇ H ₁₀ O ₂	126,06808	C ₆ H ₁₂ O ₃	132,07864	C ₉ H ₁₅ N	137,12045	C ₆ H ₅ ClO ₂	143,99781
C ₆ H ₁₀ N ₂ O	126,07931	C ₅ H ₁₂ N ₂ O ₂	132,08988	C ₇ H ₃ ClO	137,98724	C ₅ H ₅ CIN ₂ O	144,00904
C ₈ H ₁₄ O	126,10446	C ₁₀ H ₁₂	132,09390	C ₆ H ₃ CIN ₂	137,99848	C ₇ H ₉ ClO	144,03419
C ₇ H ₁₄ N ₂	126,11570	C ₇ H ₁₆ O ₂	132,11503	C ₅ H ₂ N ₂ O ₃	138,00654	C ₆ H ₉ CIN ₂	144,04543
C ₉ H ₁₈	126,14085	C ₆ H ₁₆ N ₂ O	132,12626	C ₄ H ₇ ClO ₃	138,00837	C ₅ H ₈ N ₂ O ₃	144,05349
C ₅ H ₂ CINO	126,98249	C ₃ CINO ₃	132,95667	C ₃ H ₇ CIN ₂ O ₂	138,01961	C ₁₀ H ₈ O	144,05752
C ₆ H ₆ CIN	127,01888	C ₄ H ₄ CINO ₂	132,99306	C ₈ H ₇ Cl	138,02363	C ₉ H ₈ N ₂	144,06875
C ₅ H ₅ NO ₃	127,02694	C ₇ H ₃ NO ₂	133,01638	C ₇ H ₆ O ₃	138,03170	C ₈ H ₁₃ Cl	144,07058
C ₆ H ₉ NO ₂	127,06333	C ₅ H ₈ CINO	133,02944	C ₆ H ₆ N ₂ O ₂	138,04293	C ₇ H ₁₂ O ₃	144,07864
C ₇ H ₁₃ NO	127,09971	C ₈ H ₇ NO	133,05276	C ₅ H ₁₁ ClO ₂	138,04476	C ₆ H ₁₂ N ₂ O ₂	144,08988
C ₈ H ₁₇ N	127,13610	C ₆ H ₁₂ CIN	133,06583	C ₄ H ₁₁ CIN ₂ O	138,05599	C ₈ H ₁₆ O ₂	144,11503
C ₅ HClO ₂	127,96651	C ₆ H ₁₁ NO ₃	133,07389	C ₈ H ₁₀ O ₂	138,06808	C ₇ H ₁₆ N ₂ O	144,12626
C ₄ HCIN ₂ O	127,97774	C ₉ H ₁₁ N	133,08915	C ₇ H ₁₀ N ₂ O	138,07931	C ₉ H ₂₀ O	144,15142
C ₆ H ₅ ClO	128,00289	C ₆ H ₁₅ NO ₂	133,11028	C ₉ H ₁₄ O	138,10446	C ₈ H ₂₀ N ₂	144,16265
C ₅ H ₅ CIN ₂	128,01413	C ₄ H ₃ ClO ₃	133,97707	C ₈ H ₁₄ N ₂	138,11570	C ₄ CINO ₃	144,95667
C ₄ H ₄ N ₂ O ₃	128,02219	C ₃ H ₃ CIN ₂ O ₂	133,98831	C ₁₀ H ₁₈	138,14085	C ₅ H ₄ CINO ₂	144,99306
C ₇ H ₉ Cl	128,03928	C ₈ H ₃ Cl	133,99233	C ₆ H ₂ CINO	138,98249	C ₆ H ₈ CINO	145,02944
C ₆ H ₈ O ₃	128,04734	C ₇ H ₂ O ₃	134,00040	C ₃ H ₆ CINO ₃	139,00362	C ₉ H ₇ NO	145,05276
C ₅ H ₈ N ₂ O ₂	128,05858	C ₆ H ₂ N ₂ O ₂	134,01163	C ₇ H ₆ CIN	139,01888	C ₇ H ₁₂ CIN	145,06583
C ₁₀ H ₈	128,06260	C ₅ H ₇ ClO ₂	134,01346	C ₆ H ₅ NO ₃	139,02694	C ₆ H ₁₁ NO ₃	145,07389
C ₇ H ₁₂ O ₂	128,08373	C ₄ H ₇ CIN ₂ O	134,02469	C ₄ H ₁₀ CINO ₂	139,04001	C ₁₀ H ₁₁ N	145,08915
C ₆ H ₁₂ N ₂ O	128,09496	C ₈ H ₆ O ₂	134,03678	C ₇ H ₉ NO ₂	139,06333	C ₇ H ₁₅ NO ₂	145,11028
C ₈ H ₁₆ O	128,12012	C ₇ H ₆ N ₂ O	134,04801	C ₈ H ₁₃ NO	139,09971	C ₈ H ₁₉ NO	145,14666
C ₇ H ₁₆ N ₂	128,13135	C ₆ H ₁₁ ClO	134,04984	C ₉ H ₁₇ N	139,13610	C ₅ H ₃ ClO ₃	145,97707
C ₉ H ₂₀	128,15650	C ₅ H ₁₁ CIN ₂	134,06108	C ₆ HClO ₂	139,96651	C ₄ H ₃ CIN ₂ O ₂	145,98831
C ₄ CINO ₂	128,96176	C ₄ H ₁₀ N ₂ O ₃	134,06914	C ₅ HCIN ₂ O	139,97774	C ₆ H ₇ ClO ₂	146,01346
C ₅ H ₄ CINO	128,99814	C ₉ H ₁₀ O	134,07316	C ₇ H ₅ ClO	140,00289	C ₅ H ₇ CIN ₂ O	146,02469
C ₆ H ₈ CIN	129,03453	C ₈ H ₁₀ N ₂	134,08440	C ₆ H ₅ CIN ₂	140,01413	C ₉ H ₆ O ₂	146,03678
C ₅ H ₇ NO ₃	129,04259	C ₇ H ₁₅ Cl	134,08623	C ₅ H ₄ N ₂ O ₃	140,02219	C ₈ H ₆ N ₂ O	146,04801
C ₉ H ₇ N	129,05785	C ₆ H ₁₄ O ₃	134,09430	C ₄ H ₉ ClO ₃	140,02402	C ₇ H ₁₁ ClO	146,04984
C ₆ H ₁₁ NO ₂	129,07898	C ₅ H ₁₄ N ₂ O ₂	134,10553	C ₃ H ₉ CIN ₂ O ₂	140,03526	C ₆ H ₁₁ CIN ₂	146,06108
C ₇ H ₁₅ NO	129,11536	C ₁₀ H ₁₄	134,10955	C ₈ H ₉ Cl	140,03928	C ₅ H ₁₀ N ₂ O ₃	146,06914
C ₈ H ₁₉ N	129,15175	C ₃ H ₂ CINO ₃	134,97232	C ₇ H ₈ O ₃	140,04734	C ₁₀ H ₁₀ O	146,07316
C ₅ H ₃ ClO ₂	129,98216	C ₇ H ₂ CIN	134,98758	C ₆ H ₈ N ₂ O ₂	140,05858	C ₉ H ₁₀ N ₂	146,08440
C ₄ H ₃ CIN ₂ O	129,99339	C ₆ HNO ₃	134,99564	C ₈ H ₁₂ O ₂	140,08373	C ₈ H ₁₅ Cl	146,08623
C ₆ H ₇ ClO	130,01854	C ₄ H ₆ CINO ₂	135,00871	C ₇ H ₁₂ N ₂ O	140,09496	C ₇ H ₁₄ O ₃	146,09430
C ₅ H ₇ CIN ₂	130,02978	C ₇ H ₅ NO ₂	135,03203	C ₉ H ₁₆ O	140,12012	C ₆ H ₁₄ N ₂ O ₂	146,10553
C ₄ H ₆ N ₂ O ₃	130,03784	C ₅ H ₁₀ CINO	135,04509	C ₈ H ₁₆ N ₂	140,13135	C ₈ H ₁₈ O ₂	146,13068
C ₉ H ₆ O	130,04186	C ₈ H ₉ NO	135,06841	C ₁₀ H ₂₀	140,15650	C ₇ H ₁₈ N ₂ O	146,14191
C ₈ H ₆ N ₂	130,05310	C ₆ H ₁₄ CIN	135,08148	C ₅ CINO ₂	140,96176	C ₄ H ₂ CINO ₃	146,97232
C ₇ H ₁₁ Cl	130,05493	C ₅ H ₁₃ NO ₃	135,08954	C ₆ H ₄ CINO	140,99814	C ₅ H ₆ CINO ₂	147,00871
C ₆ H ₁₀ O ₃	130,06300	C ₉ H ₁₃ N	135,10480	C ₃ H ₈ CINO ₃	141,01927	C ₈ H ₅ NO ₂	147,03203
C ₅ H ₁₀ N ₂ O ₂	130,07423	C ₇ HCIO	135,97159	C ₇ H ₈ CIN	141,03453	C ₆ H ₁₀ CINO	147,04509
C ₁₀ H ₁₀	130,07825	C ₆ HCIN ₂	135,98283	C ₆ H ₇ NO ₃	141,04259	C ₉ H ₉ NO	147,06841
C ₇ H ₁₄ O ₂	130,09938	C ₅ N ₂ O ₃	135,99089	C ₇ H ₁₁ NO ₂	141,07898	C ₇ H ₁₄ CIN	147,08148
C ₆ H ₁₄ N ₂ O	130,11061	C ₄ H ₅ ClO ₃	135,99272	C ₈ H ₁₅ NO	141,11536	C ₆ H ₁₃ NO ₃	147,08954
C ₈ H ₁₈ O	130,13576	C ₃ H ₅ CIN ₂ O ₂	136,00396	C ₉ H ₁₉ N	141,15175	C ₁₀ H ₁₃ N	147,10480
C ₇ H ₁₈ N ₂	130,14700	C ₈ H ₅ Cl	136,00798	C ₆ H ₃ ClO ₂	141,98216	C ₇ H ₁₇ NO ₂	147,12593
C ₄ H ₂ CINO ₂	130,97741	C ₇ H ₄ O ₃	136,01605	C ₅ H ₃ CIN ₂ O	141,99339	C ₃ HCIN ₂ O ₃	147,96757
C ₅ H ₆ CINO	131,01379	C ₆ H ₄ N ₂ O ₂	136,02728	C ₇ H ₇ ClO	142,01854	C ₅ H ₅ ClO ₃	147,99272
C ₈ H ₅ NO	131,03711	C ₅ H ₉ ClO ₂	136,02911	C ₆ H ₇ CIN ₂	142,02978	C ₄ H ₅ CIN ₂ O ₂	148,00396
C ₆ H ₁₀ CIN	131,05018	C ₄ H ₉ CIN ₂ O	136,04034	C ₅ H ₆ N ₂ O ₃	142,03784	C ₉ H ₅ Cl	148,00798
C ₅ H ₉ NO ₃	131,05824	C ₈ H ₈ O ₂	136,05243	C ₈ H ₁₁ Cl	142,05493	C ₈ H ₄ O ₃	148,01605
C ₉ H ₉ N	131,07350	C ₇ H ₈ N ₂ O	136,06366	C ₇ H ₁₀ O ₃	142,06300	C ₇ H ₄ N ₂ O ₂	148,02728
C ₆ H ₁₃ NO ₂	131,09463	C ₆ H ₁₃ ClO	136,06549	C ₆ H ₁₀ N ₂ O ₂	142,07423	C ₆ H ₉ ClO ₂	148,02911

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C ₅ H ₉ CIN ₂ O	148,04034	C ₈ H ₈ CIN	153,03453	C ₇ H ₁₃ NO ₃	159,08954	C ₁₀ H ₁₆ N ₂	164,13135
C ₈ H ₈ O ₂	148,05243	C ₇ H ₇ NO ₃	153,04259	C ₈ H ₁₇ NO ₂	159,12593	C ₈ H ₄ CINO	164,99814
C ₈ H ₈ N ₂ O	148,06366	C ₅ H ₁₂ CINO ₂	153,05566	C ₄ HCIN ₂ O ₃	159,96757	C ₅ H ₈ CINO ₃	165,01927
C ₇ H ₁₃ CIO	148,06549	C ₈ H ₁₁ NO ₂	153,07898	C ₆ H ₅ CIO ₃	159,99272	C ₉ H ₈ CIN	165,03453
C ₆ H ₁₃ CIN ₂	148,07673	C ₉ H ₁₅ NO	153,11536	C ₅ H ₅ CIN ₂ O ₂	160,00396	C ₈ H ₇ NO ₃	165,04259
C ₅ H ₁₂ N ₂ O ₃	148,08479	C ₁₀ H ₁₉ N	153,15175	C ₇ H ₉ CIO ₂	160,02911	C ₆ H ₁₂ CINO ₂	165,05566
C ₁₀ H ₁₂ O	148,08881	C ₇ H ₃ CIO ₂	153,98216	C ₆ H ₉ CIN ₂ O	160,04034	C ₉ H ₁₁ NO ₂	165,07898
C ₉ H ₁₂ N ₂	148,10005	C ₆ H ₃ CIN ₂ O	153,99339	C ₁₀ H ₈ O ₂	160,05243	C ₇ H ₁₆ CINO	165,09204
C ₈ H ₁₇ Cl	148,10188	C ₃ H ₇ CIN ₂ O ₃	154,01452	C ₉ H ₈ N ₂ O	160,06366	C ₁₀ H ₁₅ NO	165,11536
C ₇ H ₁₆ O ₃	148,10994	C ₈ H ₇ CIO	154,01854	C ₈ H ₁₃ CIO	160,06549	C ₈ H ₃ CIO ₂	165,98216
C ₆ H ₁₆ N ₂ O ₂	148,12118	C ₇ H ₇ CIN ₂	154,02978	C ₇ H ₁₃ CIN ₂	160,07673	C ₇ H ₃ CIN ₂ O	165,99339
C ₄ H ₄ CINO ₃	148,98797	C ₆ H ₆ N ₂ O ₃	154,03784	C ₆ H ₁₂ N ₂ O ₃	160,08479	C ₄ H ₇ CIN ₂ O ₃	166,01452
C ₈ H ₄ CIN	149,00323	C ₅ H ₁₁ CIO ₃	154,03967	C ₁₀ H ₁₂ N ₂	160,10005	C ₉ H ₇ CIO	166,01854
C ₇ H ₃ NO ₃	149,01129	C ₄ H ₁₁ CIN ₂ O ₂	154,05091	C ₉ H ₁₇ Cl	160,10188	C ₈ H ₇ CIN ₂	166,02978
C ₅ H ₈ CINO ₂	149,02436	C ₉ H ₁₁ Cl	154,05493	C ₈ H ₁₆ O ₃	160,10994	C ₇ H ₆ N ₂ O ₃	166,03784
C ₈ H ₇ NO ₂	149,04768	C ₈ H ₁₀ O ₃	154,06300	C ₇ H ₁₆ N ₂ O ₂	160,12118	C ₆ H ₁₁ CIO ₃	166,03967
C ₆ H ₁₂ CINO	149,06074	C ₇ H ₁₀ N ₂ O ₂	154,07423	C ₉ H ₂₀ O ₂	160,14633	C ₅ H ₁₁ CIN ₂ O ₂	166,05091
C ₉ H ₁₁ NO	149,08406	C ₉ H ₁₄ O ₂	154,09938	C ₈ H ₂₀ N ₂ O	160,15756	C ₁₀ H ₁₁ Cl	166,05493
C ₇ H ₁₆ CIN	149,09713	C ₈ H ₁₄ N ₂ O	154,11061	C ₅ H ₄ CINO ₃	160,98797	C ₉ H ₁₀ O ₃	166,06300
C ₆ H ₁₅ NO ₃	149,10519	C ₁₀ H ₁₈ O	154,13576	C ₆ H ₈ CINO ₂	161,02436	C ₈ H ₁₀ N ₂ O ₂	166,07423
C ₁₀ H ₁₅ N	149,12045	C ₉ H ₁₈ N ₂	154,14700	C ₉ H ₇ NO ₂	161,04768	C ₇ H ₁₅ CIO ₂	166,07606
C ₃ H ₃ CIN ₂ O ₃	149,98322	C ₆ H ₂ CINO ₂	154,97741	C ₇ H ₁₂ CINO	161,06074	C ₆ H ₁₅ CIN ₂ O	166,08729
C ₈ H ₃ CIO	149,98724	C ₇ H ₆ CINO	155,01379	C ₁₀ H ₁₁ NO	161,08406	C ₁₀ H ₁₄ O ₂	166,09938
C ₇ H ₃ CIN ₂	149,99848	C ₄ H ₁₀ CINO ₃	155,03492	C ₆ H ₁₆ CIN	161,09713	C ₉ H ₁₄ N ₂ O	166,11061
C ₉ H ₂ N ₂ O ₃	150,00654	C ₈ H ₁₀ CIN	155,05018	C ₇ H ₁₅ NO ₃	161,10519	C ₁₀ H ₁₈ N ₂	166,14700
C ₈ H ₇ CIO ₃	150,00837	C ₇ H ₉ NO ₃	155,05824	C ₈ H ₁₉ NO ₂	161,14158	C ₇ H ₂ CINO ₂	166,97741
C ₄ H ₇ CIN ₂ O ₂	150,01961	C ₈ H ₁₃ NO ₂	155,09463	C ₄ H ₃ CIN ₂ O ₃	161,98322	C ₈ H ₆ CINO	167,01379
C ₉ H ₇ Cl	150,02363	C ₉ H ₁₇ NO	155,13101	C ₆ H ₇ CIO ₃	162,00837	C ₅ H ₁₀ CINO ₃	167,03492
C ₈ H ₆ O ₃	150,03170	C ₆ HCIO ₃	155,96142	C ₅ H ₇ CIN ₂ O ₂	162,01961	C ₉ H ₁₀ CIN	167,05018
C ₇ H ₆ N ₂ O ₂	150,04293	C ₅ HCIN ₂ O ₂	155,97266	C ₁₀ H ₇ Cl	162,02363	C ₈ H ₉ NO ₃	167,05824
C ₆ H ₁₁ CIO ₂	150,04476	C ₇ H ₅ CIO ₂	155,99781	C ₉ H ₆ O ₃	162,03170	C ₆ H ₁₄ CINO ₂	167,07131
C ₅ H ₁₁ CIN ₂ O	150,05599	C ₆ H ₅ CIN ₂ O	156,00904	C ₈ H ₆ N ₂ O ₂	162,04293	C ₉ H ₁₃ NO ₂	167,09463
C ₉ H ₁₀ O ₂	150,06808	C ₈ H ₉ CIN ₂ O ₃	156,03017	C ₇ H ₁₁ CIO ₂	162,04476	C ₁₀ H ₁₇ NO	167,13101
C ₈ H ₁₀ N ₂ O	150,07931	C ₈ H ₉ CIO	156,03419	C ₆ H ₁₁ CIN ₂ O	162,05599	C ₇ HCIO ₃	167,96142
C ₇ H ₁₅ CIO	150,08114	C ₇ H ₉ CIN ₂	156,04543	C ₁₀ H ₁₀ O ₂	162,06808	C ₆ HCIN ₂ O ₂	167,97266
C ₆ H ₁₅ CIN ₂	150,09238	C ₆ H ₈ N ₂ O ₃	156,05349	C ₉ H ₁₀ N ₂ O	162,07931	C ₈ H ₅ CIO ₂	167,99781
C ₅ H ₁₄ N ₂ O ₃	150,10044	C ₉ H ₁₃ Cl	156,07058	C ₈ H ₁₅ CIO	162,08114	C ₇ H ₅ CIN ₂ O	168,00904
C ₁₀ H ₁₄ O	150,10446	C ₈ H ₁₂ O ₃	156,07864	C ₇ H ₁₅ CIN ₂	162,09238	C ₄ H ₉ CIN ₂ O ₃	168,03017
C ₉ H ₁₄ N ₂	150,11570	C ₇ H ₁₂ N ₂ O ₂	156,08988	C ₆ H ₁₄ N ₂ O ₃	162,10044	C ₉ H ₉ CIO	168,03419
C ₇ H ₂ CINO	150,98249	C ₉ H ₁₆ O ₂	156,11503	C ₁₀ H ₁₄ N ₂	162,11570	C ₈ H ₉ CIN ₂	168,04543
C ₄ H ₆ CINO ₃	151,00362	C ₈ H ₁₆ N ₂ O	156,12626	C ₉ H ₁₉ Cl	162,11753	C ₇ H ₆ N ₂ O ₃	168,05349
C ₈ H ₆ CIN	151,01888	C ₁₀ H ₂₀ O	156,15142	C ₈ H ₁₈ O ₃	162,12560	C ₆ H ₁₃ CIO ₃	168,05532
C ₇ H ₅ NO ₃	151,02694	C ₉ H ₂₀ N ₂	156,16265	C ₇ H ₁₈ N ₂ O ₂	162,13683	C ₅ H ₁₃ CIN ₂ O ₂	168,06656
C ₅ H ₁₀ CINO ₂	151,04001	C ₅ CINO ₃	156,95667	C ₅ H ₆ CINO ₃	163,00362	C ₁₀ H ₁₃ Cl	168,07058
C ₈ H ₉ NO ₂	151,06333	C ₆ H ₄ CINO ₂	156,99306	C ₉ H ₆ CIN	163,01888	C ₉ H ₁₂ O ₃	168,07864
C ₆ H ₁₄ CINO	151,07639	C ₇ H ₈ CINO	157,02944	C ₈ H ₅ NO ₃	163,02694	C ₈ H ₁₂ N ₂ O ₂	168,08988
C ₉ H ₁₃ NO	151,09971	C ₈ H ₁₂ CIN	157,06583	C ₆ H ₁₀ CINO ₂	163,04001	C ₁₀ H ₁₆ O ₂	168,11503
C ₁₀ H ₁₇ N	151,13610	C ₇ H ₁₁ NO ₃	157,07389	C ₉ H ₉ NO ₂	163,06333	C ₉ H ₁₆ N ₂ O	168,12626
C ₇ HCIO ₂	151,96651	C ₈ H ₁₅ NO ₂	157,11028	C ₇ H ₁₄ CINO	163,07639	C ₁₀ H ₂₀ N ₂	168,16265
C ₆ HCIN ₂ O	151,97774	C ₉ H ₁₉ NO	157,14666	C ₁₀ H ₁₃ NO	163,09971	C ₆ CINO ₃	168,95667
C ₃ H ₅ CIN ₂ O ₃	151,99887	C ₆ H ₃ CIO ₃	157,97707	C ₈ H ₁₈ CIN	163,11278	C ₇ H ₄ CINO ₂	168,99306
C ₈ H ₅ CIO	152,00289	C ₅ H ₃ CIN ₂ O ₂	157,98831	C ₇ H ₁₇ NO ₃	163,12084	C ₈ H ₈ CINO	169,02944
C ₇ H ₅ CIN ₂	152,01413	C ₇ H ₇ CIO ₂	158,01346	C ₄ H ₅ CIN ₂ O ₃	163,99887	C ₅ H ₁₂ CINO ₃	169,05057
C ₆ H ₄ N ₂ O ₃	152,02219	C ₆ H ₇ CIN ₂ O	158,02469	C ₉ H ₅ CIO	164,00289	C ₉ H ₁₂ CIN	169,06583
C ₅ H ₉ CIO ₃	152,02402	C ₈ H ₁₁ CIO	158,04984	C ₈ H ₅ CIN ₂	164,01413	C ₈ H ₁₁ NO ₃	169,07389
C ₄ H ₉ CIN ₂ O ₂	152,03526	C ₇ H ₁₁ CIN ₂	158,06108	C ₇ H ₄ N ₂ O ₃	164,02219	C ₉ H ₁₅ NO ₂	169,11028
C ₈ H ₉ Cl	152,03928	C ₈ H ₁₀ N ₂ O ₃	158,06914	C ₆ H ₉ CIO ₃	164,02402	C ₁₀ H ₁₉ NO	169,14666
C ₈ H ₈ O ₃	152,04734	C ₁₀ H ₁₀ N ₂	158,08440	C ₅ H ₉ CIN ₂ O ₂	164,03526	C ₇ H ₃ CIO ₃	169,97707
C ₇ H ₈ N ₂ O ₂	152,05858	C ₉ H ₁₅ Cl	158,08623	C ₁₀ H ₉ Cl	164,03928	C ₆ H ₃ CIN ₂ O ₂	169,98831
C ₆ H ₁₃ CIO ₂	152,06041	C ₈ H ₁₄ O ₃	158,09430	C ₉ H ₈ O ₃	164,04734	C ₈ H ₇ CIO ₂	170,01346
C ₅ H ₁₃ CIN ₂ O	152,07164	C ₇ H ₁₄ N ₂ O ₂	158,10553	C ₈ H ₈ N ₂ O ₂	164,05858	C ₇ H ₇ CIN ₂ O	170,02469
C ₉ H ₁₂ O ₂	152,08373	C ₉ H ₁₈ O ₂	158,13068	C ₇ H ₁₃ CIO ₂	164,06041	C ₄ H ₁₁ CIN ₂ O ₃	170,04582
C ₈ H ₁₂ N ₂ O	152,09496	C ₈ H ₁₈ N ₂ O	158,14191	C ₆ H ₁₃ CIN ₂ O	164,07164	C ₉ H ₁₁ CIO	170,04984
C ₁₀ H ₁₆ O	152,12012	C ₅ H ₂ CINO ₃	158,97232	C ₁₀ H ₁₂ O ₂	164,08373	C ₈ H ₁₁ CIN ₂	170,06108
C ₉ H ₁₆ N ₂	152,13135	C ₆ H ₆ CINO ₂	159,00871	C ₉ H ₁₂ N ₂ O	164,09496	C ₇ H ₁₀ N ₂ O ₃	170,06914
C ₆ CINO ₂	152,96176	C ₇ H ₁₀ CINO	159,04509	C ₈ H ₁₇ CIO	164,09679	C ₁₀ H ₁₅ Cl	170,08623
C ₇ H ₄ CINO	152,99814	C ₁₀ H ₉ NO	159,06841	C ₇ H ₁₇ CIN ₂	164,10803	C ₉ H ₁₄ O ₃	170,09430
C ₄ H ₈ CINO ₃	153,01927	C ₈ H ₁₄ CIN	159,08148	C ₆ H ₁₆ N ₂ O ₃	164,11609	C ₈ H ₁₄ N ₂ O ₂	170,10553

MF	Exact mass	MF	Exact mass	MF	Exact mass	MF	Exact mass
C ₁₀ H ₁₈ O ₂	170,13068	C ₁₀ H ₁₁ NO ₂	177,07898	C ₁₀ H ₁₄ CIN	183,08148	C ₈ H ₁₄ CINO ₂	191,07131
C ₉ H ₁₈ N ₂ O	170,14191	C ₈ H ₁₆ CINO	177,09204	C ₉ H ₁₃ NO ₃	183,08954	C ₉ H ₁₈ CINO	191,10769
C ₆ H ₂ CINO ₃	170,97232	C ₉ H ₂₀ CIN	177,12843	C ₁₀ H ₁₇ NO ₂	183,12593	C ₆ H ₉ CIN ₂ O ₃	192,03017
C ₇ H ₆ CINO ₂	171,00871	C ₈ H ₁₉ NO ₃	177,13649	C ₆ HCIN ₂ O ₃	183,96757	C ₁₀ H ₉ CIN ₂	192,04543
C ₈ H ₁₀ CINO	171,04509	C ₈ H ₇ CIN ₂ O ₃	178,01452	C ₈ H ₅ CIO ₃	183,99272	C ₉ H ₈ N ₂ O ₃	192,05349
C ₉ H ₁₄ CIN	171,08148	C ₁₀ H ₇ CIO	178,01854	C ₇ H ₅ CIN ₂ O ₂	184,00396	C ₈ H ₁₃ CIO ₃	192,05532
C ₈ H ₁₃ NO ₃	171,08954	C ₉ H ₇ CIN ₂	178,02978	C ₉ H ₉ CIO ₂	184,02911	C ₇ H ₁₃ CIN ₂ O ₂	192,06656
C ₉ H ₁₇ NO ₂	171,12593	C ₈ H ₆ N ₂ O ₃	178,03784	C ₈ H ₉ CIN ₂ O	184,04034	C ₁₀ H ₁₂ N ₂ O ₂	192,08988
C ₅ HCIN ₂ O ₃	171,96757	C ₇ H ₁₁ CIO ₃	178,03967	C ₅ H ₁₃ CIN ₂ O ₃	184,06147	C ₉ H ₁₇ CIO ₂	192,09171
C ₇ H ₅ CIO ₃	171,99272	C ₆ H ₁₁ CIN ₂ O ₂	178,05091	C ₁₀ H ₁₃ CIO	184,06549	C ₈ H ₁₇ CIN ₂ O	192,10294
C ₆ H ₅ CIN ₂ O ₂	172,00396	C ₁₀ H ₁₀ O ₃	178,06300	C ₉ H ₁₃ CIN ₂	184,07673	C ₈ H ₂₀ N ₂ O ₃	192,14739
C ₈ H ₉ CIO ₂	172,02911	C ₉ H ₁₀ N ₂ O ₂	178,07423	C ₈ H ₁₂ N ₂ O ₃	184,08479	C ₁₀ H ₈ CINO	193,02944
C ₇ H ₉ CIN ₂ O	172,04034	C ₈ H ₁₅ CIO ₂	178,07606	C ₁₀ H ₁₆ O ₃	184,10994	C ₇ H ₁₂ CINO ₃	193,05057
C ₉ H ₁₃ CIO	172,06549	C ₇ H ₁₅ CIN ₂ O	178,08729	C ₉ H ₁₆ N ₂ O ₂	184,12118	C ₁₀ H ₁₁ NO ₃	193,07389
C ₈ H ₁₃ CIN ₂	172,07673	C ₁₀ H ₁₄ N ₂ O	178,11061	C ₁₀ H ₂₀ N ₂ O	184,15756	C ₈ H ₁₆ CINO ₂	193,08696
C ₇ H ₁₂ N ₂ O ₃	172,08479	C ₉ H ₁₉ CIO	178,11244	C ₇ H ₄ CINO ₃	184,98797	C ₉ H ₂₀ CINO	193,12334
C ₁₀ H ₁₇ Cl	172,10188	C ₈ H ₁₉ CIN ₂	178,12368	C ₈ H ₈ CINO ₂	185,02436	C ₁₀ H ₇ CIO ₂	194,01346
C ₉ H ₁₆ O ₃	172,10994	C ₇ H ₁₈ N ₂ O ₃	178,13174	C ₉ H ₁₂ CINO	185,06074	C ₉ H ₇ CIN ₂ O	194,02469
C ₈ H ₁₆ N ₂ O ₂	172,12118	C ₉ H ₆ CINO	179,01379	C ₁₀ H ₁₆ CIN	185,09713	C ₆ H ₁₁ CIN ₂ O ₃	194,04582
C ₁₀ H ₂₀ O ₂	172,14633	C ₆ H ₁₀ CINO ₃	179,03492	C ₉ H ₁₅ NO ₃	185,10519	C ₁₀ H ₁₁ CIN ₂	194,06108
C ₉ H ₂₀ N ₂ O	172,15756	C ₁₀ H ₁₀ CIN	179,05018	C ₁₀ H ₁₉ NO ₂	185,14158	C ₉ H ₁₀ N ₂ O ₃	194,06914
C ₆ H ₄ CINO ₃	172,98797	C ₉ H ₉ NO ₃	179,05824	C ₆ H ₃ CIN ₂ O ₃	185,98322	C ₈ H ₁₅ CINO ₃	194,07097
C ₇ H ₈ CINO ₂	173,02436	C ₇ H ₁₄ CINO ₂	179,07131	C ₈ H ₇ CIO ₃	186,00837	C ₇ H ₁₅ CIN ₂ O ₂	194,08221
C ₈ H ₁₂ CINO	173,06074	C ₁₀ H ₁₃ NO ₂	179,09463	C ₇ H ₇ CIN ₂ O ₂	186,01961	C ₁₀ H ₁₄ N ₂ O ₂	194,10553
C ₉ H ₁₆ CIN	173,09713	C ₈ H ₁₈ CINO	179,10769	C ₉ H ₁₁ CIO ₂	186,04476	C ₉ H ₁₉ CIO ₂	194,10736
C ₈ H ₁₅ NO ₃	173,10519	C ₉ H ₅ CIO ₂	179,99781	C ₈ H ₁₁ CIN ₂ O	186,05599	C ₈ H ₁₉ CIN ₂ O	194,11859
C ₉ H ₁₉ NO ₂	173,14158	C ₈ H ₅ CIN ₂ O	180,00904	C ₁₀ H ₁₅ CIO	186,08114	C ₉ H ₆ CINO ₂	195,00871
C ₅ H ₃ CIN ₂ O ₃	173,98322	C ₅ H ₉ CIN ₂ O ₃	180,03017	C ₉ H ₁₅ CIN ₂	186,09238	C ₁₀ H ₁₀ CINO	195,04509
C ₇ H ₇ CIO ₃	174,00837	C ₁₀ H ₉ CIO	180,03419	C ₈ H ₁₄ N ₂ O ₃	186,10044	C ₇ H ₁₄ CINO ₃	195,06622
C ₆ H ₇ CIN ₂ O ₂	174,01961	C ₉ H ₉ CIN ₂	180,04543	C ₁₀ H ₁₈ O ₃	186,12560	C ₁₀ H ₁₃ NO ₃	195,08954
C ₈ H ₁₁ CIO ₂	174,04476	C ₈ H ₈ N ₂ O ₃	180,05349	C ₉ H ₁₈ N ₂ O ₂	186,13683	C ₈ H ₁₈ CINO ₂	195,10261
C ₇ H ₁₁ CIN ₂ O	174,05599	C ₇ H ₁₃ CIO ₃	180,05532	C ₇ H ₆ CINO ₃	187,00362	C ₉ H ₅ CIO ₃	195,99272
C ₁₀ H ₁₀ N ₂ O	174,07931	C ₆ H ₁₃ CIN ₂ O ₂	180,06656	C ₈ H ₁₀ CINO ₂	187,04001	C ₈ H ₅ CIN ₂ O ₂	196,00396
C ₉ H ₁₅ CIO	174,08114	C ₁₀ H ₁₂ O ₃	180,07864	C ₉ H ₁₄ CINO	187,07639	C ₁₀ H ₉ CIO ₂	196,02911
C ₈ H ₁₅ CIN ₂	174,09238	C ₉ H ₁₂ N ₂ O ₂	180,08988	C ₁₀ H ₁₈ CIN	187,11278	C ₉ H ₉ CIN ₂ O	196,04034
C ₇ H ₁₄ N ₂ O ₃	174,10044	C ₈ H ₁₇ CIO ₂	180,09171	C ₉ H ₁₇ NO ₃	187,12084	C ₆ H ₁₃ CIN ₂ O ₃	196,06147
C ₁₀ H ₁₉ Cl	174,11753	C ₇ H ₁₇ CIN ₂ O	180,10294	C ₆ H ₅ CIN ₂ O ₃	187,99887	C ₁₀ H ₁₃ CIN ₂	196,07673
C ₉ H ₁₈ O ₃	174,12560	C ₁₀ H ₁₆ N ₂ O	180,12626	C ₈ H ₉ CIO ₃	188,02402	C ₉ H ₁₂ N ₂ O ₃	196,08479
C ₈ H ₁₈ N ₂ O ₂	174,13683	C ₆ H ₄ CINO ₂	180,99306	C ₇ H ₉ CIN ₂ O ₂	188,03526	C ₈ H ₁₇ CIO ₃	196,08662
C ₆ H ₆ CINO ₃	175,00362	C ₉ H ₈ CINO	181,02944	C ₉ H ₁₃ CIO ₂	188,06041	C ₇ H ₁₇ CIN ₂ O ₂	196,09786
C ₇ H ₁₀ CINO ₂	175,04001	C ₆ H ₁₂ CINO ₃	181,05057	C ₈ H ₁₃ CIN ₂ O	188,07164	C ₁₀ H ₁₆ N ₂ O ₂	196,12118
C ₁₀ H ₉ NO ₂	175,06333	C ₁₀ H ₁₂ CIN	181,06583	C ₁₀ H ₁₇ CIO	188,09679	C ₈ H ₄ CINO ₃	196,98797
C ₈ H ₁₄ CINO	175,07639	C ₉ H ₁₁ NO ₃	181,07389	C ₉ H ₁₇ CIN ₂	188,10803	C ₉ H ₈ CINO ₂	197,02436
C ₉ H ₁₈ CIN	175,11278	C ₇ H ₁₆ CINO ₂	181,08696	C ₈ H ₁₆ N ₂ O ₃	188,11609	C ₁₀ H ₁₂ CINO	197,06074
C ₈ H ₁₇ NO ₃	175,12084	C ₁₀ H ₁₅ NO ₂	181,11028	C ₁₀ H ₂₀ O ₃	188,14124	C ₇ H ₁₆ CINO ₃	197,08187
C ₅ H ₅ CIN ₂ O ₃	175,99887	C ₈ H ₃ CIO ₃	181,97707	C ₉ H ₂₀ N ₂ O ₂	188,15248	C ₁₀ H ₁₅ NO ₃	197,10519
C ₇ H ₉ CIO ₃	176,02402	C ₇ H ₃ CIN ₂ O ₂	181,98831	C ₇ H ₈ CINO ₃	189,01927	C ₇ H ₃ CIN ₂ O ₃	197,98322
C ₆ H ₉ CIN ₂ O ₂	176,03526	C ₉ H ₇ CIO ₂	182,01346	C ₈ H ₁₂ CINO ₂	189,05566	C ₉ H ₇ CIO ₃	198,00837
C ₁₀ H ₈ O ₃	176,04734	C ₈ H ₇ CIN ₂ O	182,02469	C ₉ H ₁₆ CINO	189,09204	C ₈ H ₇ CIN ₂ O ₂	198,01961
C ₉ H ₈ N ₂ O ₂	176,05858	C ₅ H ₁₁ CIN ₂ O ₃	182,04582	C ₁₀ H ₂₀ CIN	189,12843	C ₁₀ H ₁₁ CIO ₂	198,04476
C ₈ H ₁₃ CIO ₂	176,06041	C ₁₀ H ₁₁ CIO	182,04984	C ₉ H ₁₉ NO ₃	189,13649	C ₉ H ₁₁ CIN ₂ O	198,05599
C ₇ H ₁₃ CIN ₂ O	176,07164	C ₉ H ₁₁ CIN ₂	182,06108	C ₆ H ₇ CIN ₂ O ₃	190,01452	C ₆ H ₁₅ CIN ₂ O ₃	198,07712
C ₁₀ H ₁₂ N ₂ O	176,09496	C ₈ H ₁₀ N ₂ O ₃	182,06914	C ₇ H ₁₁ CIO ₃	190,03967	C ₁₀ H ₁₅ CIN ₂	198,09238
C ₉ H ₁₇ CIO	176,09679	C ₇ H ₁₅ CIO ₃	182,07097	C ₇ H ₁₁ CIN ₂ O ₂	190,05091	C ₉ H ₁₄ N ₂ O ₃	198,10044
C ₈ H ₁₇ CIN ₂	176,10803	C ₆ H ₁₅ CIN ₂ O ₂	182,08221	C ₁₀ H ₁₀ N ₂ O ₂	190,07423	C ₁₀ H ₁₈ N ₂ O ₂	198,13683
C ₇ H ₁₆ N ₂ O ₃	176,11609	C ₁₀ H ₁₄ O ₃	182,09430	C ₉ H ₁₅ CIO ₂	190,07606	C ₈ H ₆ CINO ₃	199,00362
C ₉ H ₂₀ O ₃	176,14124	C ₉ H ₁₄ N ₂ O ₂	182,10553	C ₈ H ₁₅ CIN ₂ O	190,08729	C ₉ H ₁₀ CINO ₂	199,04001
C ₈ H ₂₀ N ₂ O ₂	176,15248	C ₁₀ H ₁₈ N ₂ O	182,14191	C ₁₀ H ₁₉ CIO	190,11244	C ₁₀ H ₁₄ CINO	199,07639
C ₆ H ₈ CINO ₃	177,01927	C ₇ H ₂ CINO ₃	182,97232	C ₉ H ₁₉ CIN ₂	190,12368	C ₁₀ H ₁₇ NO ₃	199,12084
C ₁₀ H ₈ CIN	177,03453	C ₈ H ₆ CINO ₂	183,00871	C ₈ H ₁₈ N ₂ O ₃	190,13174	C ₇ H ₅ CIN ₂ O ₃	199,99887
C ₉ H ₇ NO ₃	177,04259	C ₉ H ₁₀ CINO	183,04509	C ₇ H ₁₀ CINO ₃	191,03492		
C ₇ H ₁₂ CINO ₂	177,05566	C ₆ H ₁₄ CINO ₃	183,06622	C ₁₀ H ₉ NO ₃	191,05824		

NATURAL ISOTOPIC ABUNDANCE

List of isotopic natural abundance of some elements

Atom	Mass	%	Atom	Mass	%	Atom	Mass	%	Atom	Mass	%
Ag	108.904755	48.161	Fe	53.939613	5.9	Nd	141.90771	27.13	Si	28.976496	4.67
Ag	106.90509	51.839	Ga	70.9247	39.892	Nd	149.92088	5.64	Si	27.976927	92.23
Al	26.981539	100	Ga	68.92558	60.108	Nd	147.91689	5.76	Sm	153.92221	22.7
Ar	39.962383	99.6	Gd	157.9241	24.84	Nd	145.91312	17.19	Sm	151.91972	26.7
Ar	37.96273	0.063	Gd	156.92395	15.65	Nd	144.91257	8.3	Sm	149.91727	7.4
Ar	35.967545	0.337	Gd	155.92212	20.47	Nd	143.91008	23.8	Sm	148.91718	13.8
As	74.92159	100	Gd	154.92262	14.8	Ne	21.991383	9.25	Sm	147.91483	11.3
Au	196.96654	100	Gd	153.92087	2.18	Ne	20.993843	0.27	Sm	146.9149	15
B	11.009305	80.1	Gd	151.91978	0.2	Ne	19.992435	90.48	Sm	143.912	3.1
B	10.012937	19.9	Gd	159.92705	21.86	Ni	61.928345	3.634	Sn	123.90527	5.79
Ba	137.90523	71.7	Ge	75.9214	7.44	Ni	60.931057	1.14	Sn	121.90344	4.63
Ba	136.9058	11.23	Ge	73.92118	35.94	Ni	59.930786	26.223	Sn	119.9022	32.59
Ba	135.90456	7.85	Ge	72.92346	7.72	Ni	57.935345	68.077	Sn	118.90331	8.58
Ba	134.90567	6.593	Ge	71.92208	27.66	Ni	63.927967	0.926	Sn	117.90161	24.22
Ba	133.90448	2.42	Ge	69.92425	21.24	Np	237.0482	100	Sn	116.902954	7.68
Ba	131.90504	0.101	H	2.014	0.015	O	17.99916	0.2	Sn	115.90175	14.53
Ba	129.90628	0.106	H	1.007825	99.985	O	16.99913	0.04	Sn	114.90335	0.36
Be	9.012182	100	He	4.0026	100	O	15.994915	99.76	Sn	113.90279	0.65
Bi	208.98038	100	He	3.01603	1.37e-06	Os	189.95844	26.4	Sn	111.90482	0.97
Br	78.918335	50.69	Hf	173.94005	0.162	Os	188.95813	16.1	Sr	87.90562	82.58
Br	80.91629	49.31	Hf	179.94655	35.1	Os	187.95586	13.3	Sr	86.90888	7
C	13.003355	1.1	Hf	178.94582	13.629	Os	186.95573	1.6	Sr	85.90926	9.86
C	12	98.9	Hf	177.9437	27.297	Os	185.95383	1.58	Sr	83.91343	0.56
Ca	45.95369	0.004	Hf	176.94322	18.606	Os	183.95248	0.02	Ta	180.948	99.998
Ca	43.95548	2.086	Hf	175.9414	5.206	Os	191.96147	41	Ta	179.94746	0.012
Ca	42.958767	0.135	Hg	203.97346	6.87	P	30.973763	100	Tb	158.92534	100
Ca	41.95862	0.647	Hg	201.97061	29.86	Pb	206.97588	22.1	Te	125.90331	18.93
Ca	39.96259	96.941	Hg	200.97028	13.18	Pb	205.97444	24.1	Te	124.904434	7.12
Ca	47.952534	0.187	Hg	199.9683	23.1	Pb	203.97302	1.4	Te	123.902824	4.79
Cd	110.90418	12.8	Hg	198.96825	16.87	Pb	207.97662	52.4	Te	122.904274	0.905
Cd	109.90301	12.49	Hg	197.96674	9.97	Pd	109.90517	11.72	Te	121.90305	2.59
Cd	107.90418	0.89	Hg	195.9658	0.15	Pd	107.90389	26.46	Te	119.904045	0.095
Cd	115.904755	7.49	Ho	164.93031	100	Pd	105.90348	27.33	Te	129.90623	33.87
Cd	113.90336	28.73	I	126.90447	100	Pd	104.90508	22.33	Te	127.904465	31.7
Cd	112.9044	12.22	In	114.90388	95.7	Pd	103.90403	11.14	Th	232.03806	100
Cd	111.902756	24.13	In	112.90406	4.3	Pd	101.90563	1.02	Ti	46.951763	7.3
Ce	141.90924	11.13	Ir	190.96059	37.3	Pr	140.90765	100	Ti	45.95263	8
Ce	139.90543	88.43	Ir	192.96292	62.7	Pt	189.95992	0.01	Ti	49.944794	5.4
Ce	137.90599	0.25	K	40.961826	6.7302	Pt	197.96786	7.2	Ti	48.947872	5.5
Ce	135.90714	0.19	K	39.964	0.0117	Pt	195.96492	25.3	Ti	47.94795	73.8
Cl	36.965904	24.23	K	38.963707	93.2581	Pt	194.96477	33.8	Ti	204.9744	70.476
Cl	34.968853	75.77	Kr	77.9204	0.35	Pt	193.96266	32.9	Ti	202.97232	29.524
Co	58.933197	100	Kr	85.910614	17.3	Pt	191.96101	0.79	Tm	168.93422	100
Cr	53.93888	2.365	Kr	83.91151	57	Rb	86.90919	27.83	V	50.943962	99.75
Cr	52.94065	9.5	Kr	82.91414	11.5	Rb	84.9118	72.17	V	49.947163	0.25
Cr	51.94051	83.79	Kr	81.91348	11.6	Re	186.95575	62.6	W	185.95436	28.6
Cr	49.946045	4.345	Kr	79.91638	2.25	Re	184.95296	37.4	W	183.95093	30.7
Cs	132.90543	100	La	138.90634	99.9088	Rh	102.9055	100	W	182.95023	14.28
Cu	62.939598	69.17	La	137.9071	0.0902	Ru	103.905426	18.6	W	181.9482	26.3
Cu	64.927795	30.83	Li	7.016003	92.5	Ru	101.90435	31.6	W	179.9467	0.12
Dy	157.92441	0.1	Li	6.015121	7.5	Ru	100.90558	17.1	Y	88.905846	100
Dy	155.92528	0.06	Lu	174.94077	97.41	Ru	99.90422	12.6	Yb	173.93886	31.8
Dy	163.92917	28.2	Lu	175.94267	2.59	Ru	98.90594	12.7	Yb	172.9382	16.12
Dy	162.92873	24.9	Mg	25.982594	11.01	Ru	97.90529	1.86	Yb	171.93637	21.9
Dy	161.92679	25.5	Mg	24.985838	10	Ru	95.9076	5.54	Yb	170.93633	14.3
Dy	160.92693	18.9	Mg	23.985043	78.99	S	35.96708	0.02	Yb	169.93475	3.05
Dy	159.92519	2.34	Mn	54.938046	100	S	33.967865	4.21	Yb	167.9339	0.13
Er	169.93546	14.9	Mo	94.90584	15.92	S	32.971455	0.75	Yb	175.94257	12.7
Er	167.93237	26.8	Mo	93.90508	9.25	S	31.97207	95.02	Zn	69.92532	0.6
Er	166.93205	22.95	Mo	91.90681	14.84	Sb	122.90421	42.64	Zn	67.92484	18.8
Er	165.93028	33.6	Mo	99.90748	9.63	Sb	120.903824	57.36	Zn	66.92713	4.1
Er	163.9292	1.61	Mo	97.9054	24.13	Sc	44.95591	100	Zn	65.92603	27.9
Er	161.92877	0.14	Mo	96.90602	9.55	Se	77.917305	23.77	Zn	63.929146	48.6
Eu	152.92122	52.2	Mo	95.90468	16.68	Se	76.919914	7.63	Zr	93.90647	17.38
Eu	150.91985	47.8	N	15.000108	0.37	Se	75.91921	9.36	Zr	91.90504	17.15
F	18.998404	100	N	14.003074	99.63	Se	73.92248	0.89	Zr	90.90565	11.22
Fe	57.933277	0.28	Na	22.989767	100	Se	81.916695	8.74	Zr	89.9047	51.45
Fe	56.935394	2.1	Nb	92.90638	100	Se	79.91652	49.61	Zr	95.90827	2.8
Fe	55.93494	91.72	Nd	142.9098	12.18	Si	29.97377	3.1			

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TABLE 11-4

Characteristic Infrared Stretching Wavenumber Ranges of Organic Molecules

Bond or functional group	$\tilde{\nu}$ (cm^{-1})	Bond or functional group	$\tilde{\nu}$ (cm^{-1})
RO—H (alcohols)	3200–3650	RC≡N (nitriles)	2220–2260
$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCO—H} \end{array}$ (carboxylic acids)	2500–3300	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCH, RCR}' \end{array}$ (aldehydes, ketones)	1690–1750
R ₂ N—H (amines)	3250–3500	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCOR}' \end{array}$ (esters)	1735–1750
RC≡C—H (alkynes)	3260–3330	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCOH} \end{array}$ (carboxylic acids)	1710–1760
$\begin{array}{c} \diagup \\ \text{C}=\text{C} \\ \diagdown \end{array}$ (alkenes)	3050–3150	$\begin{array}{c} \diagup \\ \text{C}=\text{C} \\ \diagdown \end{array}$ (alkenes)	1620–1680
$\begin{array}{c} \\ \text{—C—H} \\ \end{array}$ (alkanes)	2840–3000	$\begin{array}{c} \\ \text{RC—OR}' \\ \end{array}$ (alcohols, ethers)	1000–1260
RC≡CH (alkynes)	2100–2260		

appendix c CHARACTERISTIC GROUP ABSORPTIONS

ALKANES

ALKENES

VINYL 

TRANS 

CIS 

VINYLDENE 

TRISUBSTITUTED 

TETRASUBSTITUTED 

CONJUGATED 

CUMULATED 

CYCLIC

ALKYNES

MONOSUBSTITUTED

DISUBSTITUTED


MONONUCLEAR AROMATICS

BENZENE

MONOSUBSTITUTED 


1,2-DISUBSTITUTED 

1,3-DISUBSTITUTED 

1,4-DISUBSTITUTED 

1,2,4-TRISUBSTITUTED 

1,2,3-TRISUBSTITUTED 

1,3,5-TRISUBSTITUTED 

ALCOHOLS AND PHENOLS

FREE OH

INTRAMOLECULAR BONDED (WEAK)

INTRAMOLECULAR BONDED (STRONG)

INTERMOLECULAR BONDED

SATURATED TERT.
HIGHLY SYMMETRICAL SEC. }

SATURATED SEC.
 α -UNSATURATED OR CYCLIC TERT. }

α -UNSATURATED SEC.
ALICYCLIC SEC. (5 OR 6-
MEMBERED RING) }

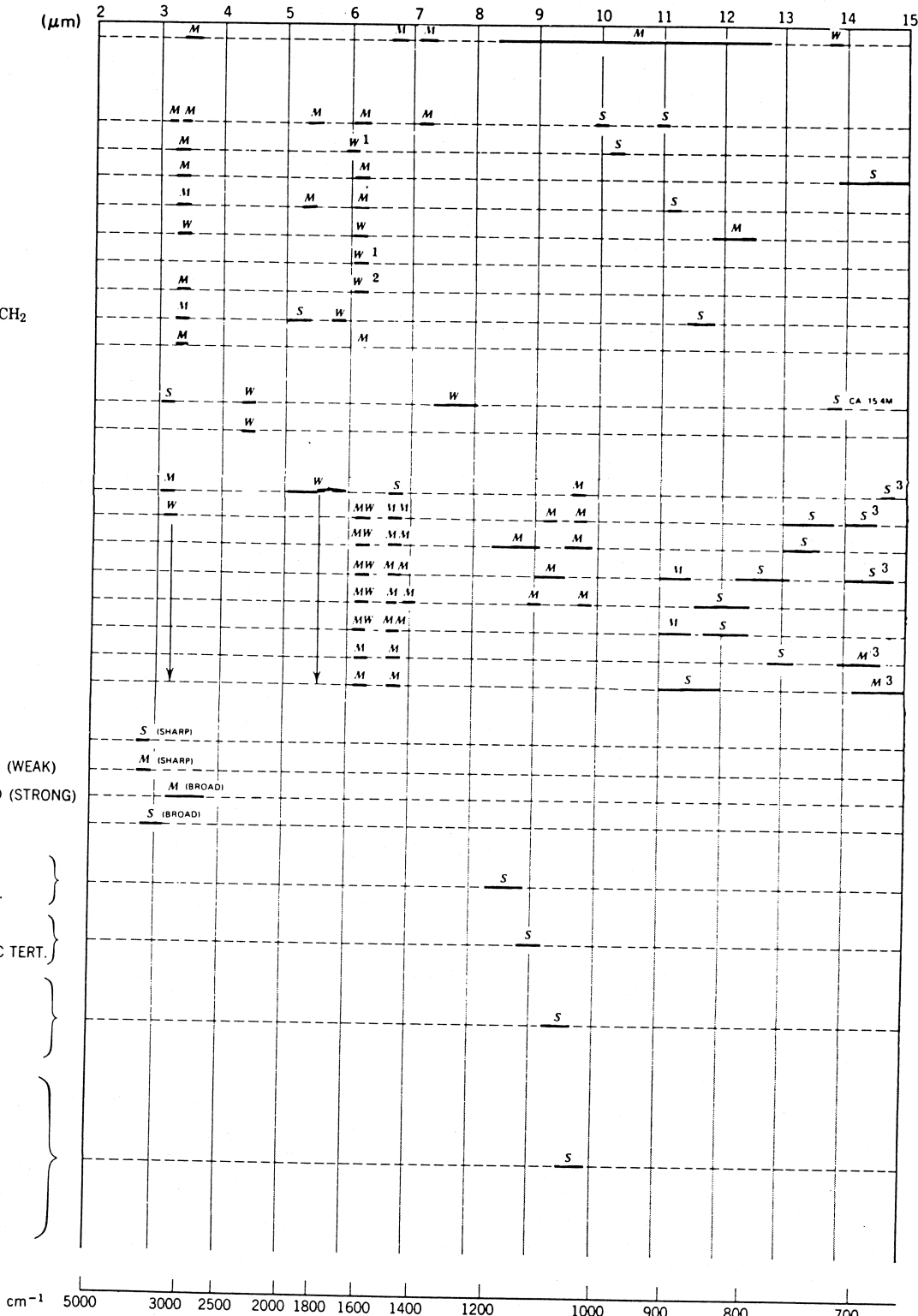
SATURATED PRIMARY }

α -UNSATURATED TERT.
 α -UNSATURATED AND
 α -BRANCHED SEC.
Di- α -UNSATURATED SEC.
ALICYCLIC SEC. (7 OR 8-
MEMBERED RING)
 α -BRANCHED AND/OR
 α -UNSATURATED PRIM. }

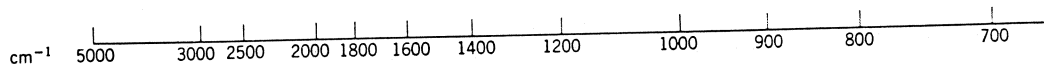
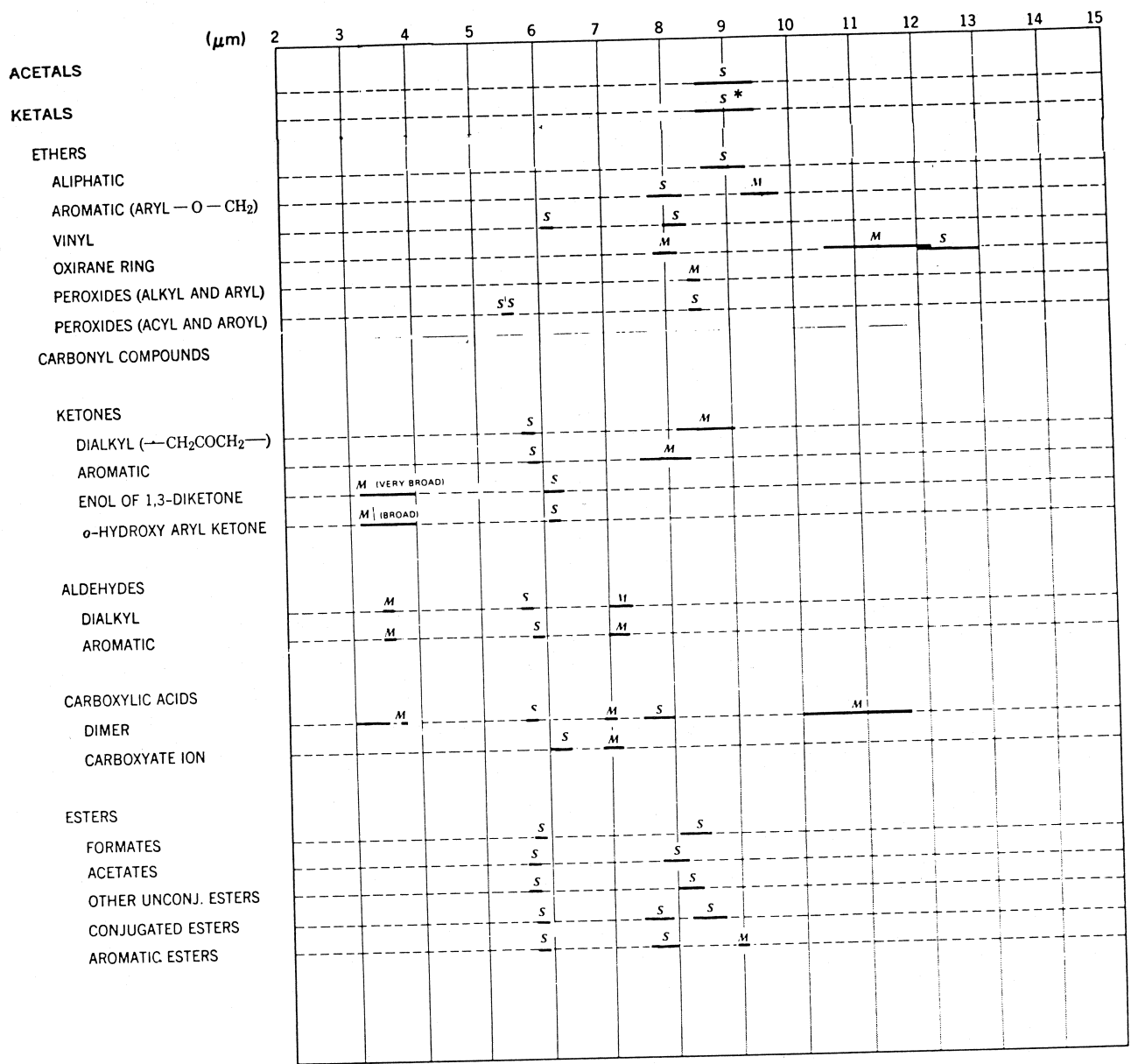
¹ May be absent

² Frequently a doublet

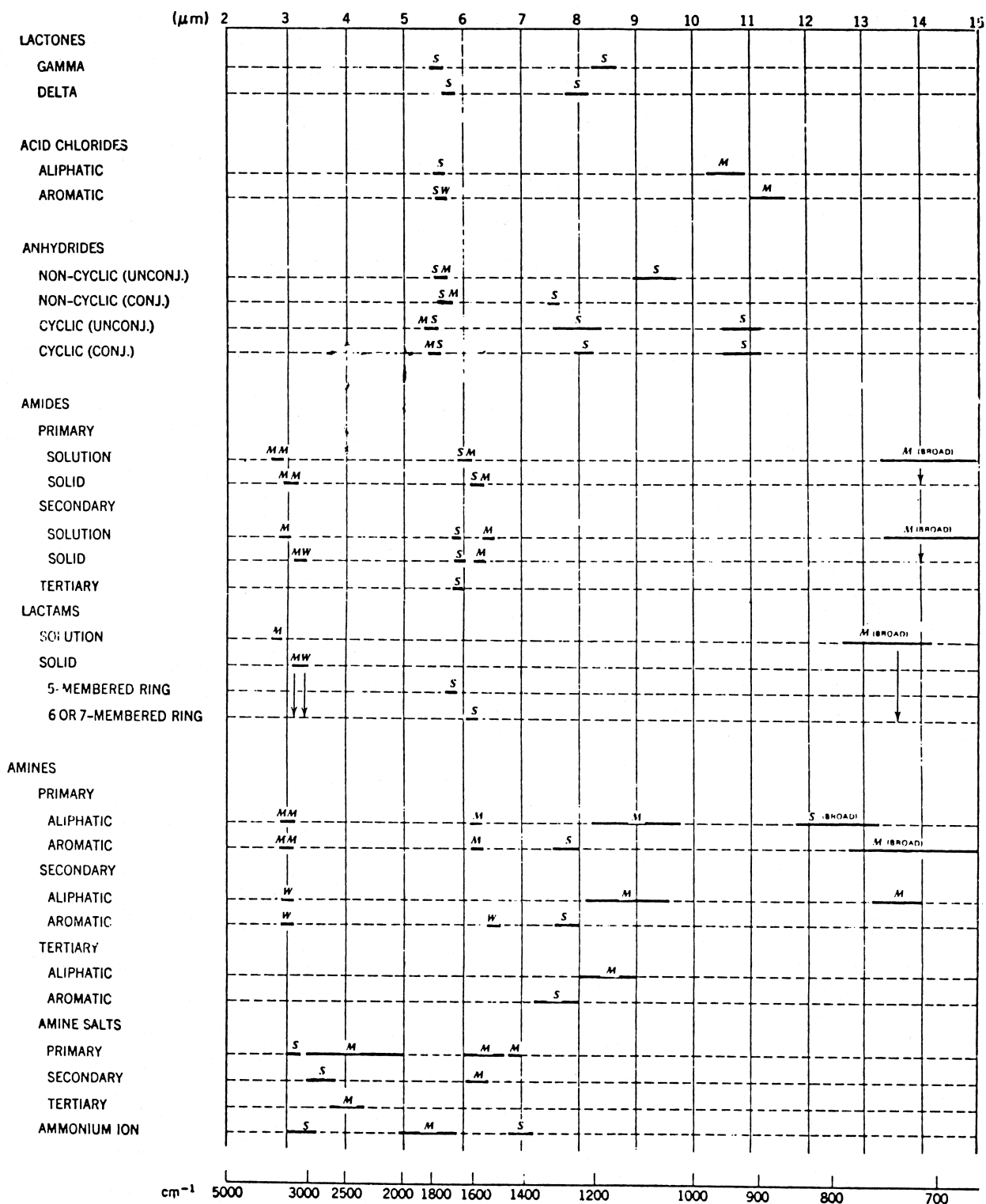
³ Ring bending bands

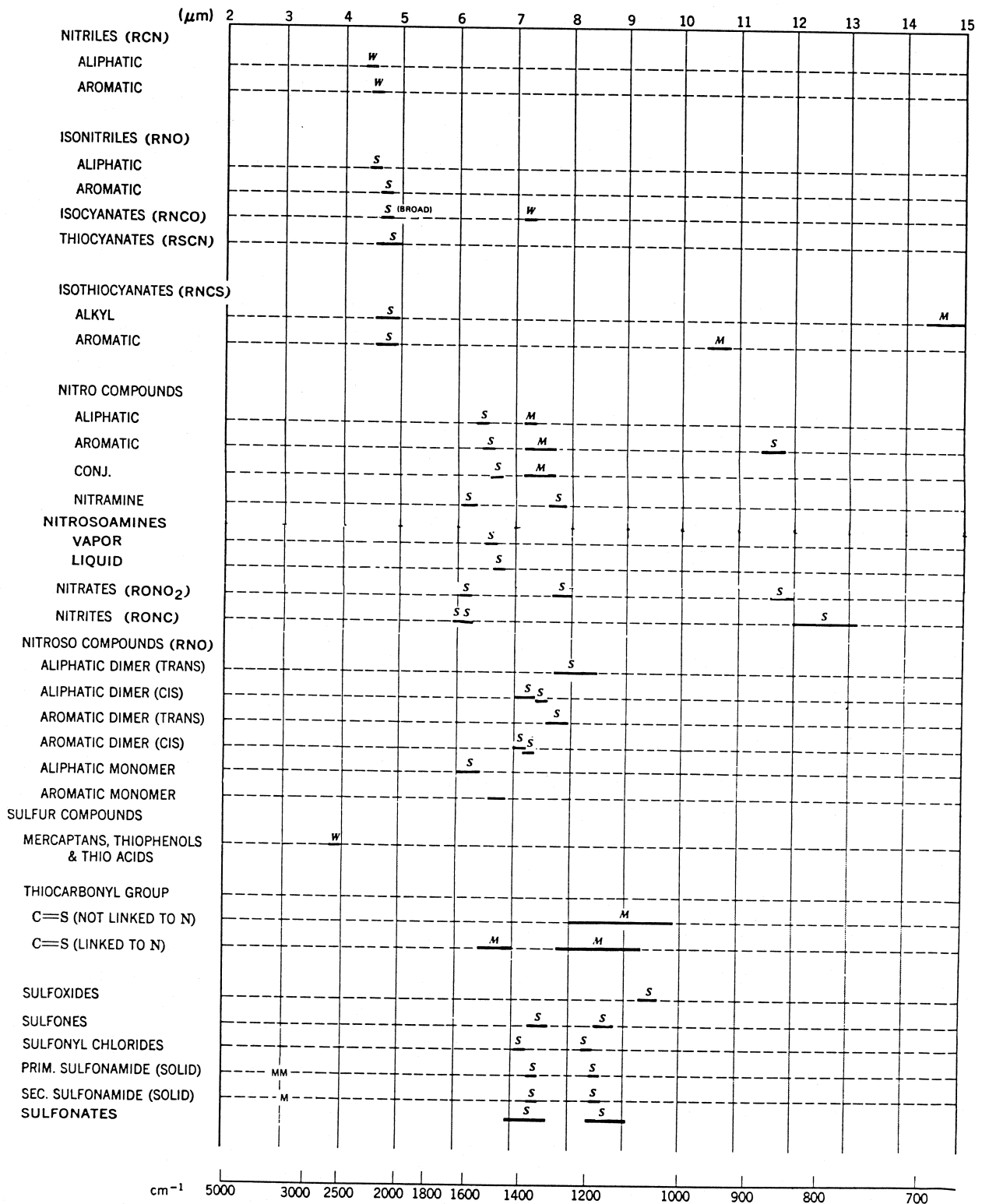


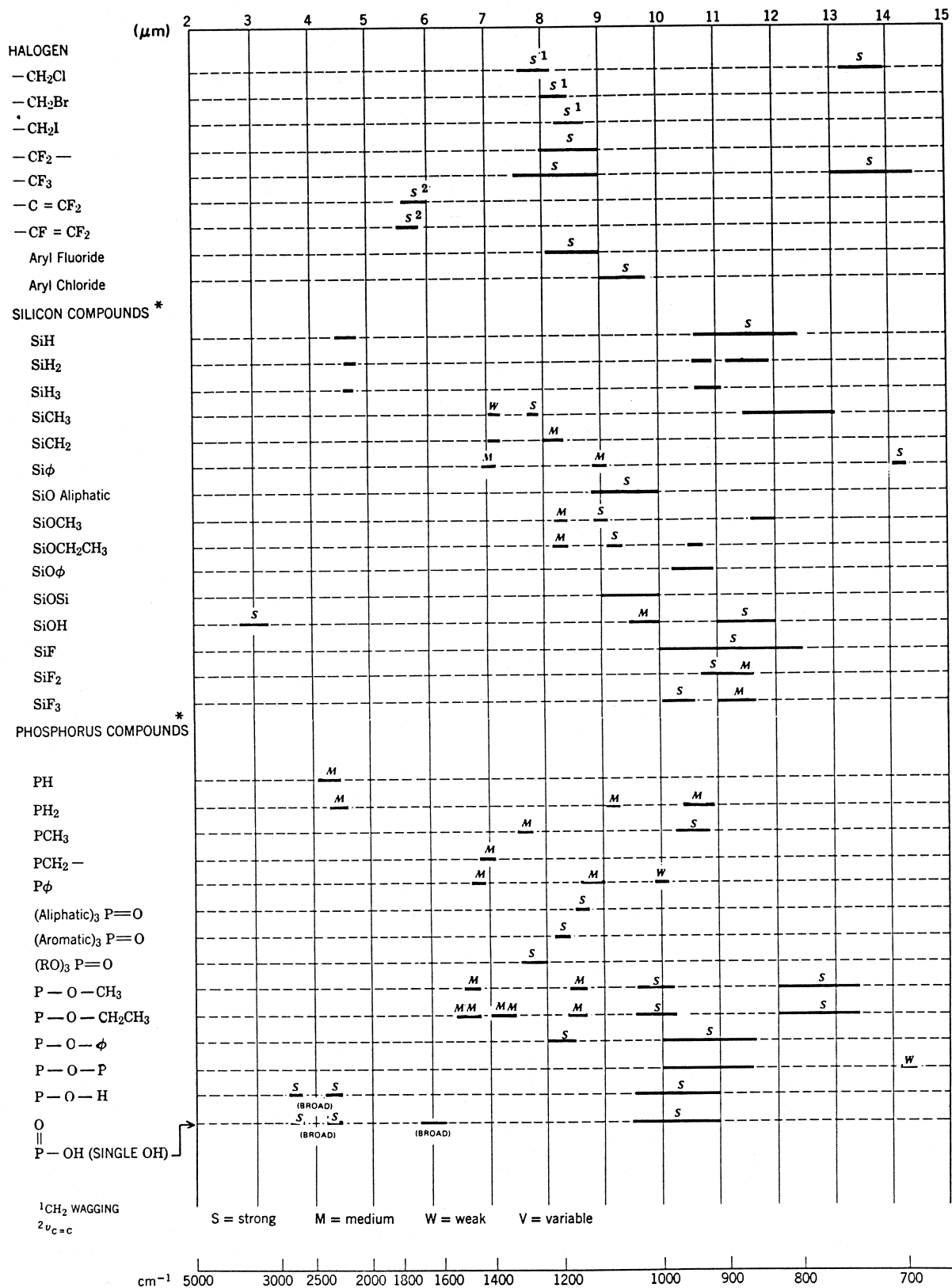
Characteristic group frequencies. The position of narrow absorption ranges is covered by a single letter indicating an average intensity. Broader absorption regions are indicated by a heavy bar. For example, a monosubstituted mononuclear aromatic may have four bands between 6 and 7 μm, three of medium intensity, and one weak.



*Three bands, sometimes a fourth band for ketals and a fifth band for acetals.





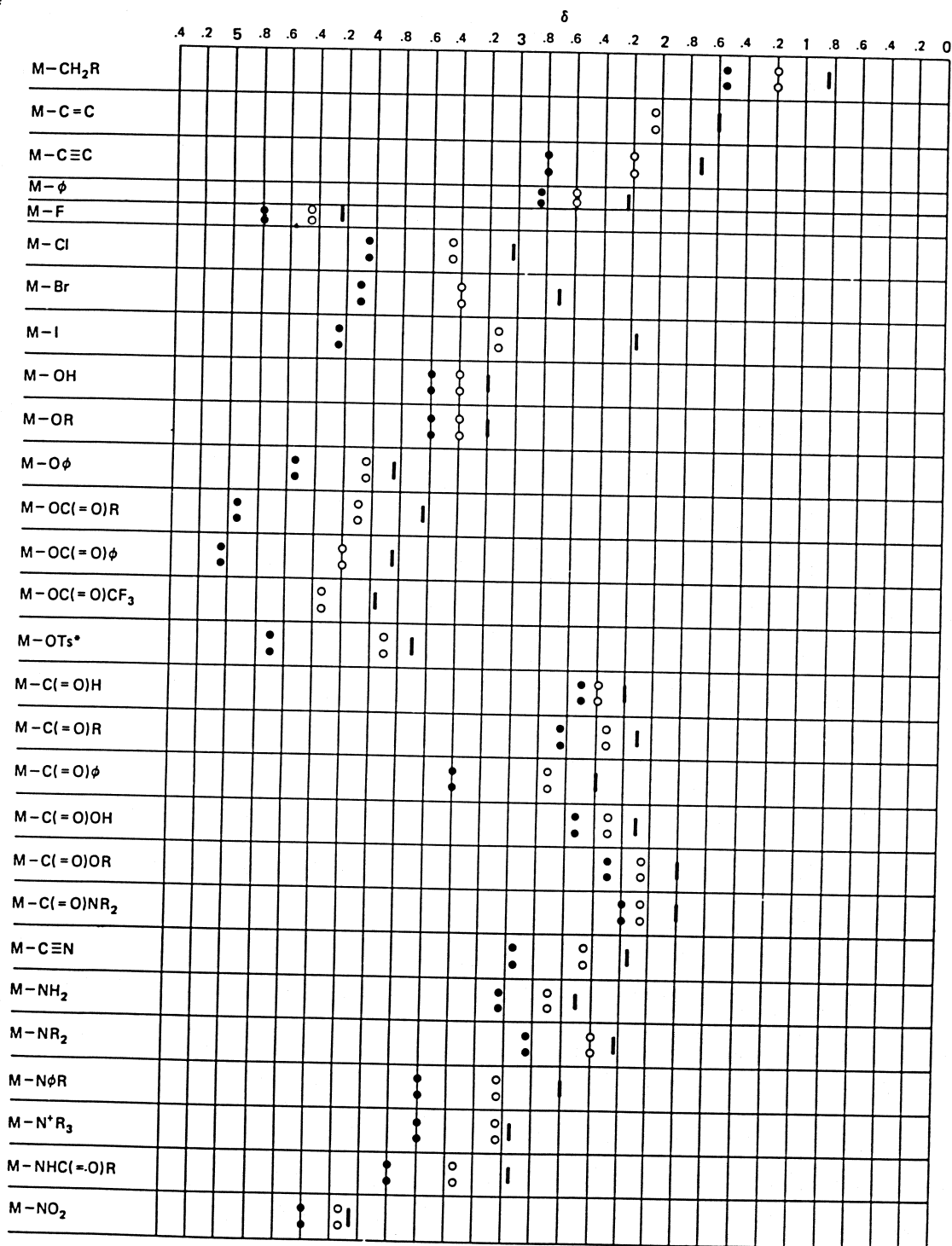


*Tables relating to these absorptions are found in Appendix E.

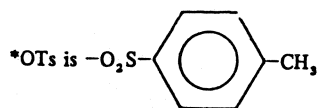
NMR

CHART 1. CHEMICAL SHIFTS OF PROTONS ON A CARBON ATOM ADJACENT (α - POSITION) TO A FUNCTIONAL GROUP IN ALIPHATIC COMPOUNDS (M-Y).

- ! M = methyl
- ⊖ M = methylene
- ⊙ M = methine



	.4	.2	5	.8	.6	.4	.2	4	.8	.6	.4	.2	3	.8	.6	.4	.2	2	.8	.6	.4	.2	1	.8	.6	.4	.2	0
M-N=C				•									○															
M-N=C=O													○															
M-O-C≡N					○																							
M-N=C=S								•		○																		
M-S-C≡N													•		○													
M-O-N=O				○																								
M-SH													•		○													
M-SR													•		○													
M-Sφ																												
M-SSR															○													
M-SOR													○															
M-SO ₂ R													○															
M-SO ₃ R																												
M-PR ₂																												
M-P ⁺ Cl ₃													○															
M-P(=O)R ₂																												
M-P(=S)R ₂															○													



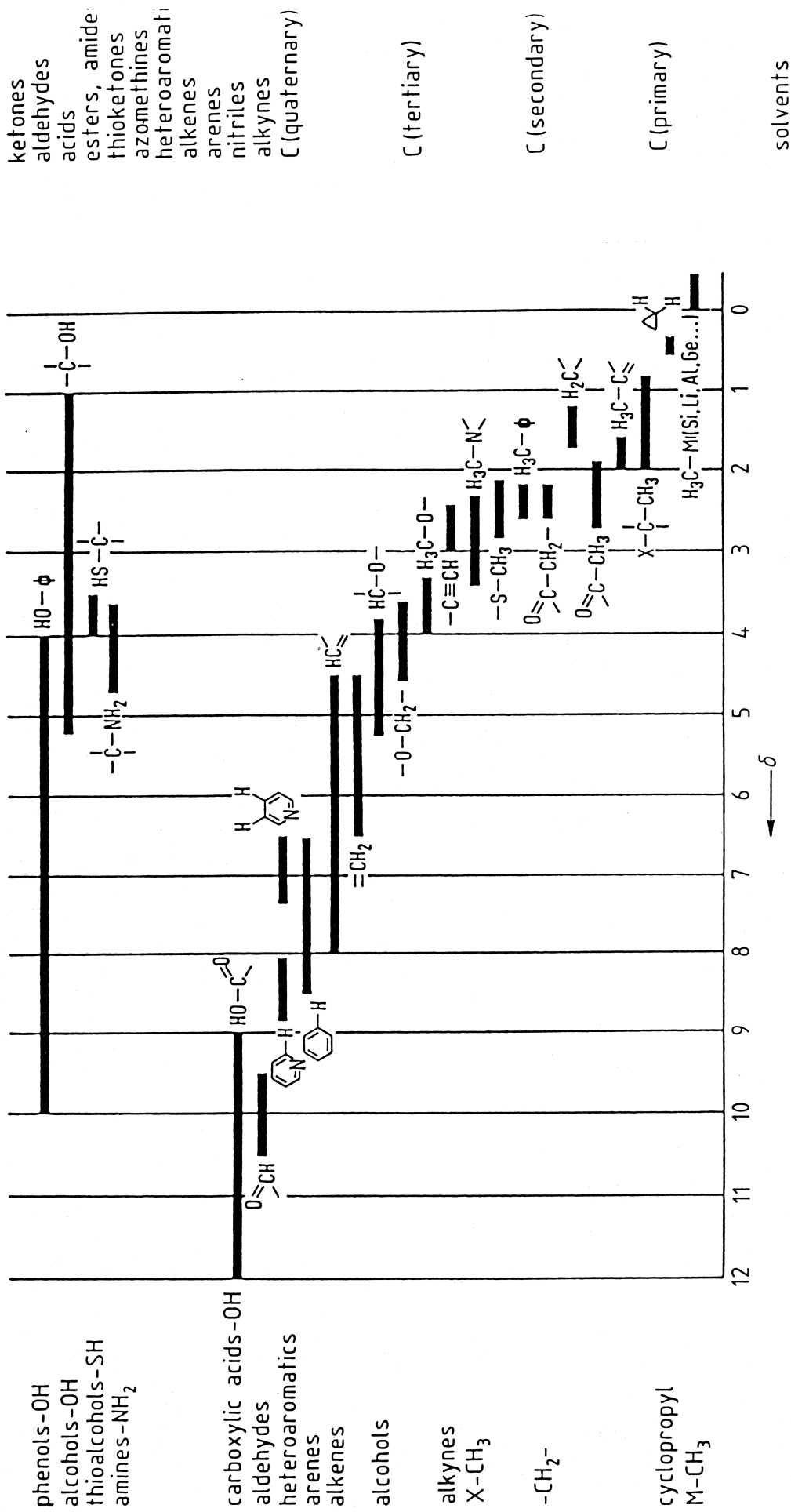


Figure 2-1.
Chemical shifts of ^1H nuclei in organic compounds.

2.1.1 Influence of the Charge Density on the Shielding

Figure 2-2.
Chemical sh

¹H-NMR

SUBSTITUTED ALKANES

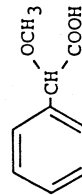
Estimation of the Chemical Shift in Polysubstituted Alkanes
(δ in ppm relative to TMS)

$$\delta_{CH_2R_1R_2} = 1.25 + \sum_1^2 z_i$$

$$\delta_{CHR_1R_2R_3} = 1.50 + \sum_1^3 z_i$$

Substituent	z_i
-alkyl	0.0
-C=C-	0.8
-C≡C-	0.9
-phenyl	1.3
-Cl	2.0
-Br	1.9
-I	1.4
-OH	1.7
-O-alkyl	1.5
-O-phenyl	2.3
-OCO-alkyl	2.7
-NH ₂	2.9
-N-alkyl ₂	1.0
-NO ₂	3.0
-S-alkyl	1.0
-CHO	1.2
-CO-alkyl	1.2
-COOH	0.8
-COO-alkyl	0.7
-CN	1.2

Example:



base value:	1.5
-O-alkyl	1.5
-COOH	0.8
-phenyl	1.3
estimated:	5.1
determined:	4.8

¹H-NMR

SUBSTITUTED ALKANES

Estimation of the ¹H-Chemical Shift of Methylene Groups $R_1CH_2R_2$
(δ in ppm relative to TMS); see H.M. Bell, L.K. Berry, E.A. Madigan,
Org. Magn. Res. 22, 693 (1984).

$$\delta_{CH_2R_1R_2} = 0.23 + z_{R_1} + z_{R_2}$$

Substituent R	z_R
-alkyl	see p. H17
-C=C-	1.33
-CECH	1.52
-C≡Calkyl	1.52
-C≡Cphenyl	1.77
-phenyl	1.85
H-F	3.15
A-Cl	2.48
L-Br	2.29
-OH	2.46
-Oalkyl	2.27
-Ophenyl	2.89
-OCOalkyl	2.98
-OCOPhenyl	3.23
-NH ₂	1.69
-NHalkyl	1.60
-N(alkyl) ₂	1.41
-NHphenyl ₂	2.15
-N(alkyl)phenyl	2.39
-NH ₃ ⁺	2.31
-NH ₂ ⁺ alkyl	2.31
-NH ₃ ⁺ (alkyl) ₂	2.46
-N ⁺ (alkyl) ₃	2.56
-NHCOalkyl	2.23
-N(alkyl)COalkyl	2.23
-NHCOPhenyl	2.33
-SH	1.63
-Salkyl	1.63
-Sphenyl	1.92
-COalkyl	1.58
-COPhenyl	2.08
-COOH	1.49
-COOalkyl	1.49
-COOPhenyl	1.74
-CONH ₂	1.39
-CON(alkyl) ₂	1.39
-CONHphenyl	1.59
-CEN	1.73

a) for CD₃SOCD₃ or CD₃SOCD₃/CDCl₃ as solvent 0.2-0.3 ppm lower values must be used.

b) for CDCl as solvent 0.3-0.5 ppm higher values must be used.

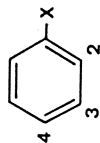
¹H-NMR

BENZENE, SUBSTITUENT EFFECTS

¹H-NMR

BENZENE, SUBSTITUENT EFFECTS

Effect of a Substituent on the Chemical Shift of the Ring-Protons in Benzene (δ in ppm relative to TMS)



$$\delta_{H_i} = 7.26 + Z_i$$

Substituent X	Z ₂	Z ₃	Z ₄
-H	0	0	0
-CH ₃	-0.20	-0.12	-0.22
-CH ₂ CH ₃	-0.14	-0.06	-0.17
-CH(CH ₃) ₂	-0.13	-0.08	-0.18
-C(CH ₃) ₃	0.02	-0.08	-0.21
-CH ₂ Cl	0.00	0.00	0.00
-CF ₃	0.32	0.14	0.20
-CCl ₃	0.64	0.13	0.10
-CH ₂ OH	-0.07	-0.07	-0.07
-CH=CH ₂	0.06	-0.03	-0.10
-CH=CH-phenyl	0.15	-0.01	-0.16
-C≡CH	0.15	-0.02	-0.01
-C≡C-phenyl	0.19	0.02	0.00
-phenyl	0.37	0.20	0.10
-F	-0.26	0.00	-0.20
-Cl	0.03	-0.02	-0.09
-Br	0.18	-0.08	-0.04
-I	0.39	-0.21	0.00
-OH	-0.56	-0.12	-0.45
-OCH ₃	-0.48	-0.09	-0.44
-OCH ₂ CH ₃	-0.46	-0.10	-0.43
-O-phenyl	-0.29	-0.05	-0.23
-OCOCH ₃	-0.25	0.03	-0.13
-CO-phenyl	-0.09	0.09	-0.08
-OSO ₂ CH ₃	-0.05	0.07	-0.01

Substituent X	Z ₂	Z ₃	Z ₄
-NH ₂	-0.75	-0.25	-0.65
-NHCH ₃	-0.80	-0.22	-0.68
-N(CH ₃) ₂	-0.66	-0.18	-0.67
-N ⁺ (CH ₃) ₃ I ⁻	0.69	0.36	0.31
-NHCOCH ₃	0.12	-0.07	-0.28
-N(CH ₃)COCH ₃	-0.16	0.05	-0.02
-NHNH ₂	-0.60	-0.08	-0.55
-N=N-phenyl	0.67	0.20	0.20
-NO	0.58	0.31	0.37
-NO ₂	0.95	0.26	0.38
-SH	-0.08	-0.16	-0.22
-SCH ₃	-0.08	-0.10	-0.24
-S-phenyl	0.06	-0.09	-0.15
-SO ₃ CH ₃	0.60	0.26	0.33
-SO ₂ Cl	0.76	0.35	0.45
-CHO	0.56	0.22	0.29
-COCH ₃	0.62	0.14	0.21
-COCH ₂ CH ₃	0.63	0.13	0.20
-COC(CH ₃) ₃	0.44	0.05	0.05
-CO-phenyl	0.47	0.13	0.22
-COOH	0.85	0.18	0.27
-COOCH ₃	0.71	0.11	0.21
-COOCH(CH ₃) ₂	0.70	0.09	0.19
-COO-phenyl	0.90	0.17	0.27
-CONH ₂	0.61	0.10	0.17
-COCl	0.84	0.22	0.36
-COBr	0.80	0.21	0.37
-CH=N-phenyl	~0.6	~0.2	~0.2
-CN	0.36	0.18	0.28
-Si(CH ₃) ₃	0.22	-0.02	-0.02
-PO(OCH ₃) ₂	0.48	0.16	0.24

¹H-NMR

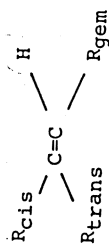
ALKENES, ADDITIVITY RULE

¹H-NMR

ALKENES, ADDITIVITY RULE

The Chemical Shift of Protons at a Double Bond
(δ in ppm relative to TMS)

$$\delta_{\text{C=CH}} = 5.25 + Z_{\text{gem}} + Z_{\text{cis}} + Z_{\text{trans}}$$



Substituent R	Z _{gem}	Z _{cis}	Z _{trans}
-H	0	0	0
-alkyl	0.45	-0.22	-0.28
-alkyl ring ¹⁾	0.69	-0.25	-0.28
-CH ₂ -aromatic	1.05	-0.29	-0.32
-CH ₂ X, X: F, Cl, Br	0.70	0.11	-0.04
-CHF ₂	0.66	0.32	0.21
-CF ₃	0.66	0.61	0.32
-CH ₂ O	0.64	-0.01	-0.02
-CH ₂ N	0.58	-0.10	-0.08
-CH ₂ S	0.71	-0.13	-0.22
-CH ₂ CO, CH ₂ CN	0.69	-0.08	-0.06
-C=C isolated	1.00	-0.09	-0.23
-C=C conjugated ²⁾	1.24	0.02	-0.05
-C≡C	0.47	0.38	0.12
-aromatic free rotation	1.38	0.36	-0.07
-aromatic fixed ³⁾	1.60	-	-0.05
-aromatic o-substituted	1.65	0.19	0.09
-F	1.54	-0.40	-1.02
-Cl	1.08	0.18	0.13
-Br	1.07	0.45	0.55
-I	1.14	0.81	0.88

- 1) The increment for "alkyl ring" is to be used if the substituent and the double bond are part of a cyclic structure.
- 2) The increment "C=C conjugated" is to be used if either the double bond or the C=C substituent is conjugated to other substituents.
- 3) The increment "aromatic, fixed" is to be used if the double bond conjugated to an aromatic ring is part of a fused ring (such as in 1,2-dihydronaphthalene).

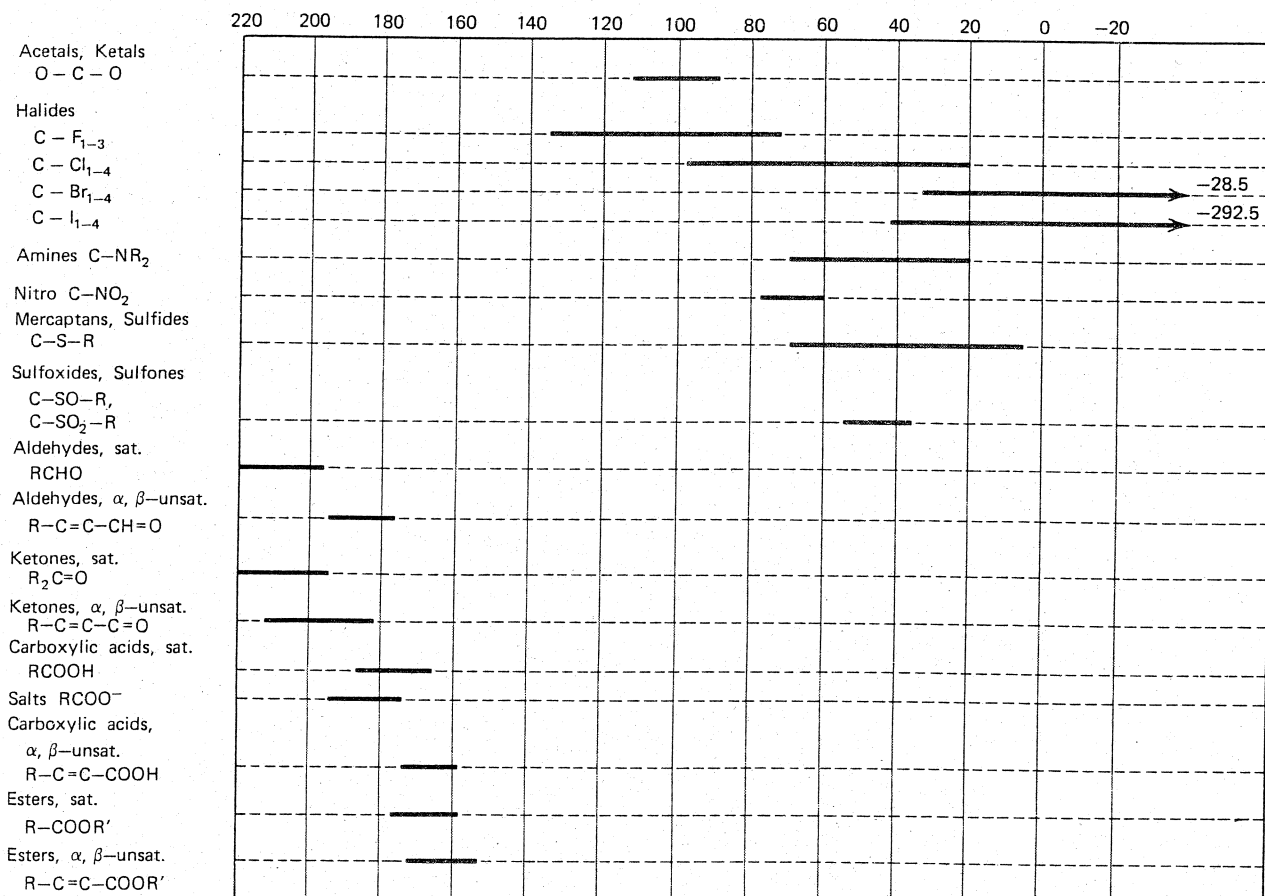
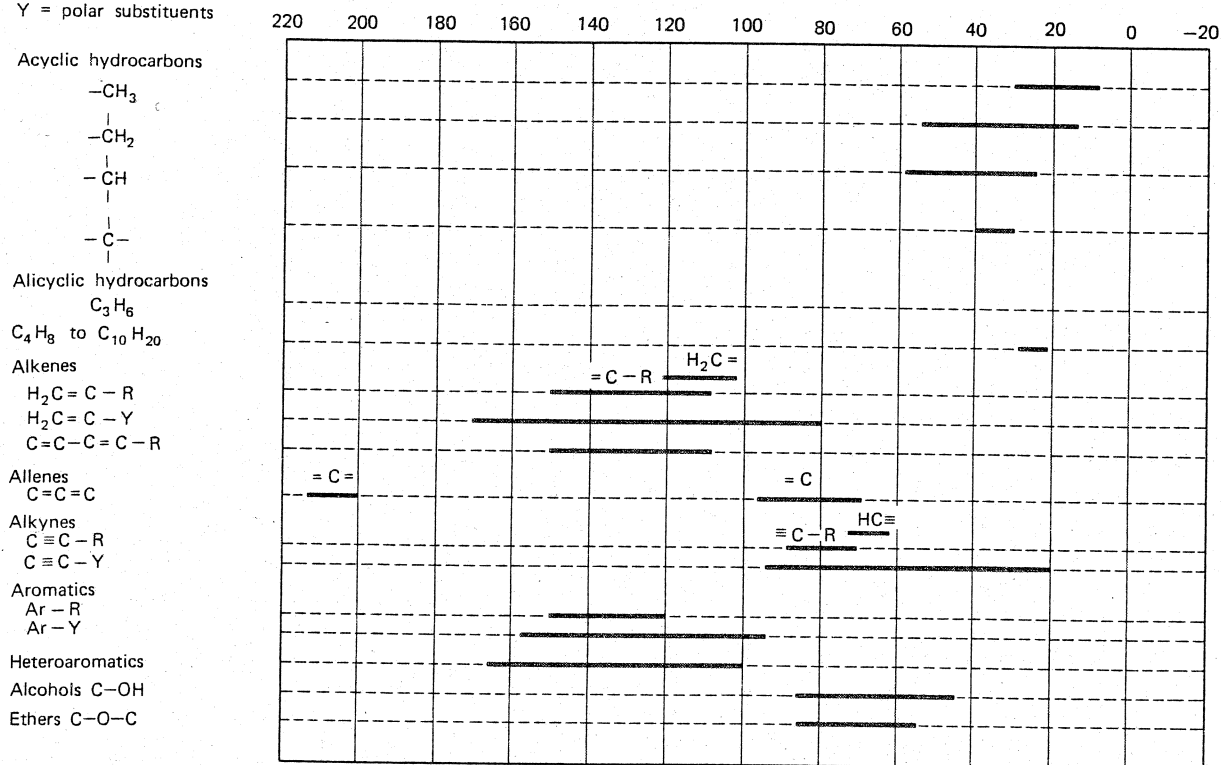
Substituent R	Z _{gem}	Z _{cis}	Z _{trans}
O			
-OR, R aliphatic	1.22	-1.07	-1.21
-OR, R unsaturated	1.21	-0.60	-1.00
-OCOR	2.11	-0.35	-0.64
-NH ₂	0.80	-1.26	-1.21
-NHS, R aliphatic	0.80	-1.26	-1.21
-NR ₂ , R aliphatic	0.80	-1.26	-1.21
-NHR, R unsaturated	1.17	-0.53	-0.99
-NRR', R unsaturated, } R' any substituent	1.17	-0.53	-0.99
-NCOR	2.08	-0.57	-0.72
-N=N-phenyl	2.39	1.11	0.67
-NO ₂	1.87	1.30	0.62
-SR	1.11	-0.29	-0.13
-SOR	1.27	0.67	0.41
-SO ₂ R	1.55	1.16	0.93
-SCOR	1.41	0.06	0.02
-SCN	0.94	0.45	0.41
-SF ₅	1.68	0.61	0.49
-CHO	1.02	0.95	1.17
-CO isolated	1.10	1.12	0.87
-CO conjugated ¹⁾	1.06	0.91	0.74
-COOH isolated	0.97	1.41	0.71
-COOH conjugated ¹⁾	0.80	0.98	0.32
-COOR isolated	0.80	1.18	0.55
-COOR conjugated ¹⁾	0.78	1.01	0.46
-CONR ₂	1.37	0.98	0.46
-COCl	1.11	1.46	1.01
-CN	0.27	0.75	0.55
-PO(OCH ₂ CH ₃) ₂	0.66	0.88	0.67
-PO(OCH ₂ CH ₃) ₂	1.33	-0.34	-0.66
S			
N			
O=C			
A			

- 1) The increment "conjugated" is to be used if either the double bond or the substituent is conjugated to additional substituents.

appendix c. ¹³C correlation chart for chemical classes.

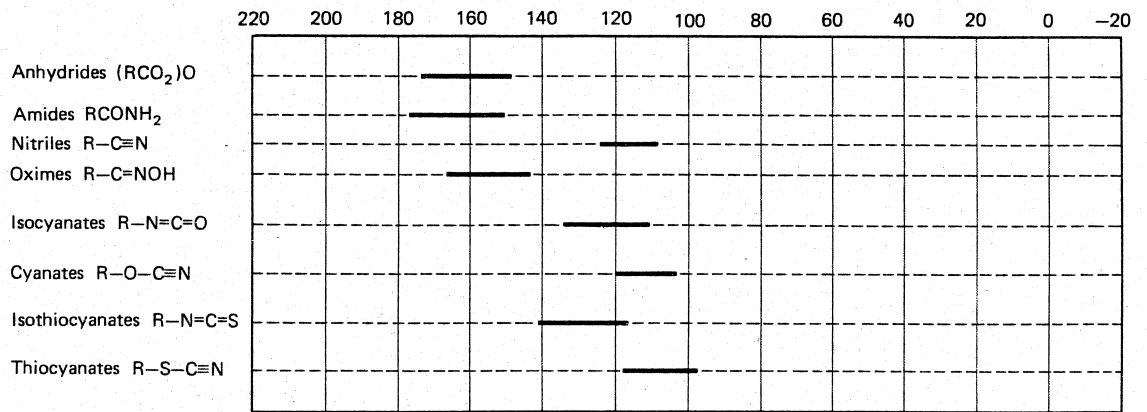
R = H or alkyl substituents
Y = polar substituents

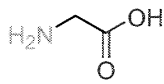
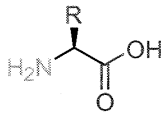
¹³C Correlation Chart for Chemical Classes



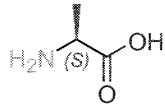
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appendix c (continued)

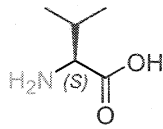




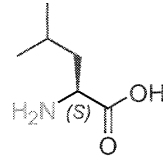
Glycine
Gly
G



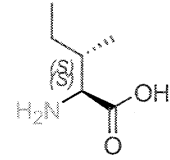
Alanine
Ala
A



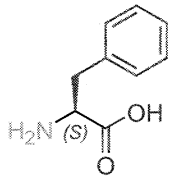
Valine
Val
V



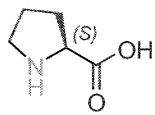
Leucine
Leu
L



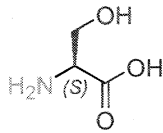
Isoleucine
Ile
I



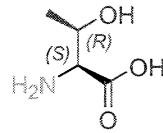
Phenylalanine
Phe
F



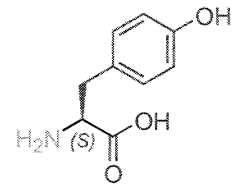
Proline
Pro
P



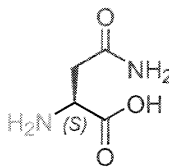
Serine
Ser
S



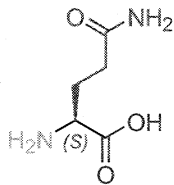
Threonine
Thr
T



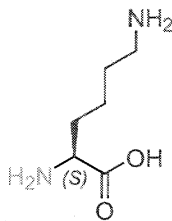
Tyrosine
Tyr
Y



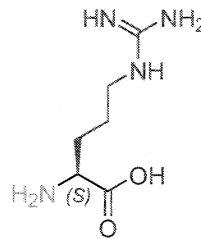
Asparagine
Asn
N



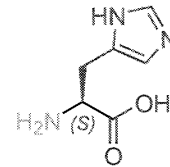
Glutamine
Gln
Q



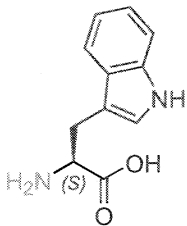
Lysine
Lys
K



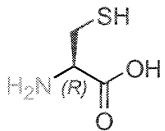
Arginine
Arg
R



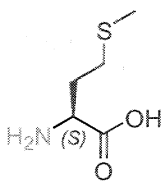
Histidine
His
H



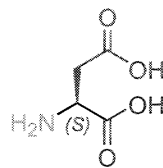
Tryptophan
Trp
W



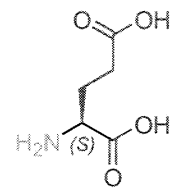
Cysteine
Cys
C



Methionine
Met
M



Aspartic acid
Asp
D



Glutamic acid
Glu
E