

# TAURANGA GIRLS’ COLLEGE

# NCEA LEVEL 3 CHEMISTRY

RESOURCE BOOKLET

## AS 91388 Demonstrate understanding of spectroscopic data in chemistry 3 credits

#### Version 1

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**IR absorptions for representative functional groups**

|  |  |  |  |
| --- | --- | --- | --- |
| **Molecular Motion** | **Wavenumber (cm−1)** | **Molecular Motion** | **Wavenumber (cm−1)** |
| N–H stretch (1 per N–H bond) | 3500–3300 | C═O stretch | 1750–1700 |
| O–H stretch | 3600–3300 | C═O stretch (amide) | 1680–1630 |
| O–H stretch (carboxylic acid) | 3400–2400 | C═C stretch | 1690–1630 |
| ═C–H stretch | 3100–3010 | N–H bend | 1640–1500 |
| C–H stretch | 2950–2800 | C–O stretch | 1320–1210 |
| C–H aldehyde stretch | ~2850 and ~2750 | C–Cl stretch | 785–540 |
| C═O stretch (acyl chlorides) | 1810–1775 | C–Br | 650–510 |

**13C NMR chemical shift (ppm) Fragments in Mass Spectrum**

|  |  |
| --- | --- |
| **Relative mass** | **Molecular ion, M+** |
| 15 | CH3+ |
| 17 | OH+ |
| 27 | C2H3+ |
| 29 | C2H5+ or CHO+ |
| 31 | OCH3+ or CH2OH+ |
| 35 & 37 | Cl+ |
| 41 | C3H5+ |
| 43 | C3H7+ |
| 45 | COOH+ |
| 59 | CH2COOH+ or COOCH3+ |
| 62 & 64 | CCH2Cl+ |
| 63 & 65 | CHCH2Cl+ |
| 79 & 81 | Br+ |

|  |  |
| --- | --- |
| **Carbon environment** | **Chemical shift (ppm)** |
| C=O (in ketones) | 200–230 |
| C=O (in aldehydes) | 190–220 |
| C=O (in acids and esters) | 150–185 |
| C=C (in alkenes) | 115–140 |
| RCO2CH2R’ (esters) | 60–80 |
| RCH2OH | 50–65 |
| RCH2Cl | 40–45 |
| RCH2Br | 30–40 |
| RCH2NH2 | 37–45 |
| R3CH | 25–35 |
| CH3CO– | 20–30 |
| R2CH2 | 16–25 |
| RCH3 | 10–15 |

**PERIODIC TABLE OF ELEMENTS**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | | 18 |
| 1 | 2 |  | | Atomic Number | |  | |  | | 1  **H**  1·0 | | Relative atomic mass | |  | |  | |  | |  | | 13 | | 14 | | 15 | | 16 | | 17 | | 2  **He**  4·0 |
| 3  **Li**  6·9 | 4  **Be**  9·0 |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | | 5  **B**  10·8 | | 6  **C**  12·0 | | 7  **N**  14·0 | | 8  **O**  16·0 | | 9  **F**  19·0 | | 10  **Ne**  20·2 |
| 11  **Na**  23·0 | 12  **Mg**  24·3 | 3 | | 4 | | 5 | | 6 | | 7 | | 8 | | 9 | | 10 | | 11 | | 12 | | 13  **Al**  27·0 | | 14  **Si**  28·1 | | 15  **P**  31·0 | | 16  **S**  32·1 | | 17  **Cl**  35·5 | | 18  **Ar**  40·0 |
| 19  **K**  39·1 | 20  **Ca**  40·1 | 21  **Sc**  45·0 | | 22  **Ti**  47·9 | | 23  **V**  50·9 | | 24  **Cr**  52·0 | | 25  **Mn**  54·9 | | 26  **Fe**  55·9 | | 27  **Co**  58·9 | | 28  **Ni**  58·7 | | 29  **Cu**  63·5 | | 30  **Zn**  65·4 | | 31  **Ga**  69·7 | | 32  **Ge**  72·6 | | 33  **As**  74·9 | | 34  **Se**  79·0 | | 35  **Br**  79·9 | | 36  **Kr**  83·8 |
| 37  **Rb**  85·5 | 38  **Sr**  87·6 | 39  **Y**  88·9 | | 40  **Zr**  91·2 | | 41  **Nb**  92·9 | | 42  **Mo**  95·9 | | 43  **Tc**  98·9 | | 44  **Ru**  101 | | 45  **Rh**  103 | | 46  **Pd**  106 | | 47  **Ag**  108 | | 48  **Cd**  112 | | 49  **In**  115 | | 50  **Sn**  119 | | 51  **Sb**  122 | | 52  **Te**  128 | | 53  **I**  127 | | 54  **Xe**  131 |
| 55  **Cs**  133 | 56  **Ba**  137 | 71  **Lu**  175 | | 72  **Hf**  179 | | 73  **Ta**  181 | | 74  **W**  184 | | 75  **Re**  186 | | 76  **Os**  190 | | 77  **Ir**  192 | | 78  **Pt**  195 | | 79  **Au**  197 | | 80  **Hg**  201 | | 81  **Tl**  204 | | 82  **Pb**  207 | | 83  **Bi**  209 | | 84  **Po**  (209) | | 85  **At**  210 | | 86  **Rn**  (222) |
| 87  **Fr**  223 | 88  **Ra**  226 | 103  **Lr**  (260) | | 104  **Rf**  (261) | | 105  **Db**  (262) | | 106  **Sg**  (263) | | 107  **Bh**  (264) | | 108  **Hs**  (265) | | 109  **Mt**  (266) | | 110  **Ds**  (271) | | 111  **Rg**  (272) | | 112  **Cn**  (277) | |  | | 114  (289) | |  | | 116  (289) | |  | |  |
|  |  |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  | |  |
| Lanthanide Series | | | 57  **La**  139 | | 58  **Ce**  140 | | 59  **Pr**  141 | | 60  **Nd**  144 | | 61  **Pm**  147 | | 62  **Sm**  150 | | 63  **Eu**  152 | | 64  **Gd**  157 | | 65  **Tb**  159 | | 66  **Dy**  163 | | 67  **Ho**  165 | | 68  **Er**  167 | | 69  **Tm**  169 | | 70  **Yb**  173 | |
| Actinide Series | | | 89  **Ac**  227 | | 90  **Th**  232 | | 91  **Pa**  231 | | 92  **U**  238 | | 93  **Np**  237 | | 94  **Pu**  (244) | | 95  **Am**  (243) | | 96  **Cm**  (247) | | 97  **Bk**  (247) | | 98  **Cf**  (251) | | 99  **Es**  (252) | | 100  **Fm**  (257) | | 101  **Md**  (258) | | 102  **No**  (259) | |