

## O1- WebCSD Selected Refcodes

The following tables highlight reffcodes that can be used for demonstration when teaching various topics.

### Functional Groups

Functional Group	Reffcode
Alkane	DUCKOB04 ETHANE01 HEPTAN02 HEXANE01 JAYDUI OCTANE01 PENTAN01 WIMTAN01 SUSJIZ
Alkene	ETHLEN10 PAPVAD
Halogenoalkane	CLCBUT CLMETH FACETC10 MBRMET10 MIMETH10
Aldehyde	DEMTEU GEVREE OVANIL
Ketone	ACETPH ANTQUO08 ANDRSO BNZQUI03 BPHENO03 GAGSIR HIXHIF05 NESCAQ
Carboxylic Acid	ACETAC07 ACRLAC02 ACSALA01 ADIPAC04 BENZAC01 CYACAC DAYNUN FACETC10 FORMAC01 YILLAG
Primary Alcohol	ADEZUF ETANOL KEDKOT LUPNIN METHOL NESCAQ QATVAI
Secondary Alcohol	BIDLOP CYOCDL DAYNUN KEDKOT NESCAQ YILLAG
Tertiary Alcohol	CITARC YIMWEW
Acyl/Acid Chloride	MUCONC10 PAMPEY
Ester	ACSALA01 BAHSUY CEBGUL COUMAR02 DAYNUN GAGSIR YARZUN03
Acetic Anhydride	JADJAA
Amides	BZAMID02 HXACAN11 JAHZEX10 MBNZAM10 PYRZIN
Primary Amine	ETDIAM12 FIGYID METAMI QABLAG
Secondary Amine	EPHEDR01 LANKUH PSEPED01 QABLAG
Tertiary Amine	CEKGUU01 KASPUQ LUPNIN DALQOW
Aromatics	BENZEN CORONE NAPHTA04 TOLUEN
Aryl Halides	ACEPOO DCLBEN03 FACFAQ
Phenol	PHENOL03
Cyclohexane	CYCHEX
Nitrile	BITVUV CADVEI CYACAC LIKSAZ

**Optical Isomers** - There are many molecules in the teaching subset that have chiral centres. The table below gives a selection of these. **The two isomers of thalidomide are THALID10 and THALID03.**

	Reffcode
1 Chiral Centre	ADRENL ALUCAL05 ASPARM08 CIVFOC10 CMPXPA DAYNUN DLASPA02 DLHIST DLMALC11 DLMETA05 DOXSIS EPHEDR01 FAKHOO GLUTAM01 IBPRAC04 LALNIN23 LASCAC02 LCYSTN22 LGLUAC01 LSERIN01 LTYROS10 LUPNIN MORPHM NEDMIS NESCAQ RERXIV SIMPEJ SUSKOG TYRPTC VALIDL VITAAC01 WIJNEI YILLAG
Multiple Chiral Centres	ABINOS ACIFEX ACIFIB ADENOS10 ADODON ALDRIN BAVLOS BOQJUM CHOCAL CHOEST20 COCAIN10 CYTIDI11 DACMOR01 DAWGOX DHPRTO DIGOXN10 DLILEU02 ESTDOL10 ESTRIO ESTRON10 FRUCTO11 GEJVEW HMFLUT10 IWESOS JAYZEO KEDKOT LTHREO01 PROGST01 PSEPED01 QNGHSU03 SUGXAU TESTOM01 THALID10 THALID03 TMZDAN10 WARFAR10 ZZZTSE01

## Geometric Isomers

Type	Refcode
Cis	ACENYL01 ALDRIN BNZQUI03 HMFLUT10 KUDWIV MALAIC10 WINCED
Trans	ABEKUN ABIKUR CADVEI INDIGO03 QETNAF WINCEB
E	BBZCPO12 CAFINE CHOCAL CUNGAT DBRING01 DEMTEU DEQZUV DERWAY DIGOXN10 FACROQ FOCLOY GAGSIR KODJES LEZHUT MUCONC UDAVIF TMCOTT VITAAC01
Z	ACIFEX ADAHAP COXDHN01 BAPLOT01 BEURID10 CHOCAL CHOEST20 COUMAR02 DACMOR01 DHRPTO PROGST01 RERXIV WOMHEM YAHSIJ

**Transition metals** - The table below highlights the refcodes for certain shapes of transition metals and their ligands. Some may have multiple types of ligand.

Type	Refcode
Linear	ACABAH
Octahedral	ACAJIX BOYHAY01 CACWOS CECZEP CECZIT CEFXOA COPGOD DUSHAA FAJXOE FOFTOK KOVSOD LOLWIS LITREL OGAZAX (YUHRIC YUHROI fac/mer isomers)
Tetrahedral	CETXOO DBBZPN FOJBUB02 FUBYIK XADQUP
Square Planar	AGOGUY DADXOW DBBZPN DEDWUE GODGIP NIMGLO10 PETKAB REJXAG TPORCP11
Other	ACEQII CEZNIE CMTUCU10 COBZAU CTPOCO DEDZUR FOJBOV01 HENNET ITETIK PEPSES
Monodentate	ACEQII BOYHAY01 CACWOS CCXAPT CEFXOA CEYXOO COBZAU COPGOD DBBZPN DEDZUR DUSHAA FOFTOK FOJBOV01 FOJBUB02 FUBYIK GODGIP KOVSOD LOLWIS OGAZAX PEPSES PETKAB XADQUP YUHRIC YUHROI
Bidentate	ACAJIX ACEQII AGOGUY BOYHAY01 FAJXOE HENNET LOLWIS LITREL NIMGLO10 PEPSES
Multidentate	CEFXOA CEZNIE CTPOCO DADXOW DEDWUE DEDZUR DUMVEM ITETIK REJXAG TPORCP11

**VSEPR shapes** - The molecules in the other category are VSEPR shapes that are affected by lone pairs.

Shape	Refcode
Linear	ACABAH IDUQED QAFPOD QIRHUU RIKTAG TPASTB
Tetrahedral	ACARBM01 CLMETH CUCEF DOGPIY GAFLAA HEJNOZ HEVRUV IYUVAZ KIPPEE LIALET01 PETKAB RIZMIW TPASTB
Trigonal Planar	APCRBP10 DOMWUX HIWQEJ IYUVAZ JAGREP TRMEIN03
Pyramidal	AWUDIF CEKGUU01 HMTNTI JOYKAJ KAXSEI
Square Planar	HEJNOZ
Octahedral	BOMQOJ DUDKUI10 HIWQEJ IYUVAZ KEFXUO NIGTOM
Trigonal Bi-pyramidal	BEJFIF FILMOC01 KUYMUM PPHOXP SOBWAH YALROS
Other	CLCHTF COXYIX GAJLEJ JASBUB PHSECL01 QEZYUQ TMTBZS YASVAP

## Macrocycles

Macrocycle	NASLOI JOJROP FOPCAO CEFXAM BIBWAL JIKJUI KAZXIU DEDWUE BECYIR CEFXOA CIFKOS CTPOCO CUSRAJ DENZUR FUJCUI GEGZOI GEJNOY GINROK HOXNND10 HOXOCD02 ITETIK JOPJIH KATLAT MAYLUU (Cryptand) OPVPFE10 PORPIN01 PVPFEO20 REJXAG TPORCP11 UFUQER
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## Amino Acids

Amino Acid	Refcode
Alanine	ALUCAL05
Asparagine	ASPARM08
Aspartic Acid	DLASPA02
Histidine	DLHIST
Alanine	LALNIN23
Cysteine	LCYSTN22
Glutamic Acid	LGLUAC01
Serine	LSERIN01
Threonine	LTHREO01
Tyrosine	LTYROS10
Tryptophan	TRYPTC
Valine	VALIDL
Arginine	WIJNEI

## Molecules of interest

Molecule	Refcode
Acetic Acid	ACETAC07
Acetylene	ACETYL03
Adenosine	ADENOS10
Benzene	BENZEN BENZEN02
Carotene	CARTEN CARTEN02
Caffeine	CAFINE
Cisplatin	CUKRAB01
Cholesterol	CHOEST20 CHOEST21
Vitamin D	CHOCAL
Citric Acid	CITARC
Cocaine	COCAIN10
Cyclohexane	CYCHEX
Ethanol	ETANOL
Ethene	ETHLEN10
Ferrocene	FEROCE18 FEROCE27
Diborane	GAFLAA
Glucose	GLUCSA
Indigo	INDIGO03
Morphine	MORPHM
Naphthalene	NAPHTA04 NAPHTA12
Vanillin	OVANIL
Phenol	PHENOL01 PHENOL03
Pyridine	PYRDNA01
Cyclopropane	QQQCIS01
C <sub>60</sub> Fullerene	SOCTOT31
Sucrose	SUCROS01
Electrophilic Addition Intermediate	DAKVUG
Electrophilic Substitution Intermediate	BAXQIA
Aspirin	ACSALA01
Nitrotoluene	NITOLU
TNT	ZZZNQS03