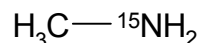


## ISOTOPES, especially DEUTERIUM

Isotopes of a given element have the same number of protons (thus are chemically the same) but different numbers of neutrons in the nucleus e.g. Carbon-12/Carbon-14. Hydrogen with a neutron in its nucleus is called Deuterium (chemical symbol D or  $^2\text{H}$ ), and Hydrogen with 2 neutrons is Tritium (T or  $^3\text{H}$ ). Although the increased mass of Deuterium and Tritium will affect their reaction rates, they are still Hydrogen from a chemical point of view.

When aspecting a compound, the presence of an isotope is indicated with the code D04 Isotope. Usually this presents no problem: the compound is aspected as normal, and D04 added, e.g.:

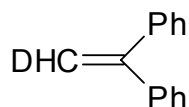
1: Methylamine made from  $^{15}\text{N}$ :



Nitrogen-15 is still nitrogen, so the functional group is still an amine. The aspects are identical to those of methylamine, with the addition of D04 Isotope:

D01	Organic
D04	Isotope
D11	Saturated aliphatic
D50	No unsaturation
D81	1 carbon in molecule
F08	Monoamine

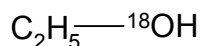
2: Deuterated diphenylethylene:



Deuterium is just a form of hydrogen, so this compound is a hydrocarbon which contains a terminal unsaturation. The aspects are identical to those of diphenylethylene, with the addition of D04 Isotope:

D01	Organic
D02	Hydrocarbon
D04	Isotope
D12	Unsaturated aliphatic
D19	Benzene ring
D32	2 rings in molecule
D76	6-membered ring
D53	Monoolefinic molecule
D58	Terminal olefinic unsaturation
D93	13-18 carbons in molecule

3: Ethanol containing  $^{18}\text{O}$

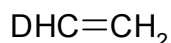


Ethanol has an R-number in the Chemicals hierarchy, but it cannot be used to describe this compound because it does not autopost D04, and additional aspects cannot be tied to R-numbers. So it has to be fully aspected:

D01	Organic
D04	Isotope
D11	Saturated aliphatic
D50	No unsaturation in molecule
D82	2 carbons in molecule
F28	Monoalcohol

The problems begin when dealing with polymer formers, which require R/G-codes. In fact they are not that difficult, you just have to bear in mind i) that isotopes do not change the *chemical structure* of a compound, and therefore do not change its overall aspecting (apart from the addition of D04 of course); and ii) that aspects can be added to a G-number, but not to an R-number. There are no R-numbers which autopost D04, so any polymer former containing an isotope will require a G-number - it is just a question of using the normal indexing rules to select the correct one.

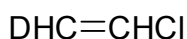
**4: Deuterated ethylene as a polymer former:**



Chemically this compound is still ethylene, but as a monomer it cannot be indexed using R00326 Ethylene. This is because R00326 does not autopost D04 Isotope, and the D04 aspect cannot be tied to an R-number. But deuterated ethylene is still an olefin, since deuterium is a form of hydrogen, so this monomer is indexed thus:

G0066 Other straight chain aliphatic monoolefinic hydrocarbon  
(autoposts D01, D02, D12, D10, D51, D53)  
D04 Isotope  
D58 Terminal olefinic unsaturation  
D82 2 carbons in molecule

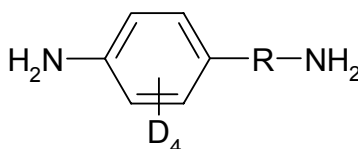
**5: Deuterated vinyl chloride as a polymer former:**



Chemically this is still vinyl chloride but, similarly to example 4, it cannot be indexed using R00338 Vinyl chloride + D04. Again, deuterium is hydrogen, so this compound is still a vinyl halide, albeit one without an R-number, so index:

G0544 Vinyl halides general  
D04 Isotope  
Cl Chlorine

**6: Look at the Diamine polymer formers hierarchy and consider this Markush compound:**

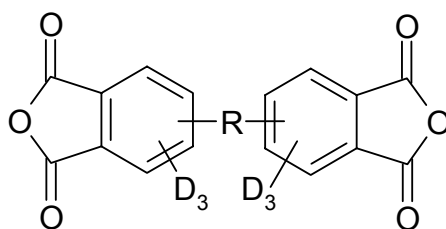


where D = deuterium, R = -O-phenylene- or a direct bond.

By the rules described above, this monomer could be a G1694 Other diaminodiphenyl ether (when R = -O-phenylene-), or a G1774 Other diaminobenzene (when R = a direct bond). By the normal indexing rules you go up the hierarchy to the lowest term that has both those codes as narrow terms, and index thus:

G1672 Diamines general  
D04 Isotope  
D19 Benzene  
D31 1 ring in molecule  
D32 2 rings in molecule  
D76 6-membered ring system  
D50 No unsaturation in molecule  
D86 6 carbons in molecule  
D92 12 carbons in molecule  
F34 Ether

7: Look at the Polybasic carboxylic anhydrides hierarchy and consider this Markush compound:



where D = deuterium, R = -CO- or direct bond.

This compound could never be R05043 Benzophenone tetracarboxylic anhydride or R12068 Biphenyl tetracarboxylic anhydride, because the presence of deuterium prohibits the use of those R-numbers. It will always be a G1434 *Other* polybasic carboxylic anhydride. But note that it is perfectly valid to aspect E33 and E34.

G1434 Other polybasic carboxylic anhydride  
D04 Isotope  
D24 Bicyclic heterocyclic  
D34 4 rings in molecule  
D77 7-9 membered ring system  
D42 1 oxygen in ring system  
D50 No unsaturation in molecule  
D93 13-18 carbons in molecule  
F23 Ketone  
E33 Benzophenone tetracarboxyli-  
E34 Biphenyl tetracarboxyli-