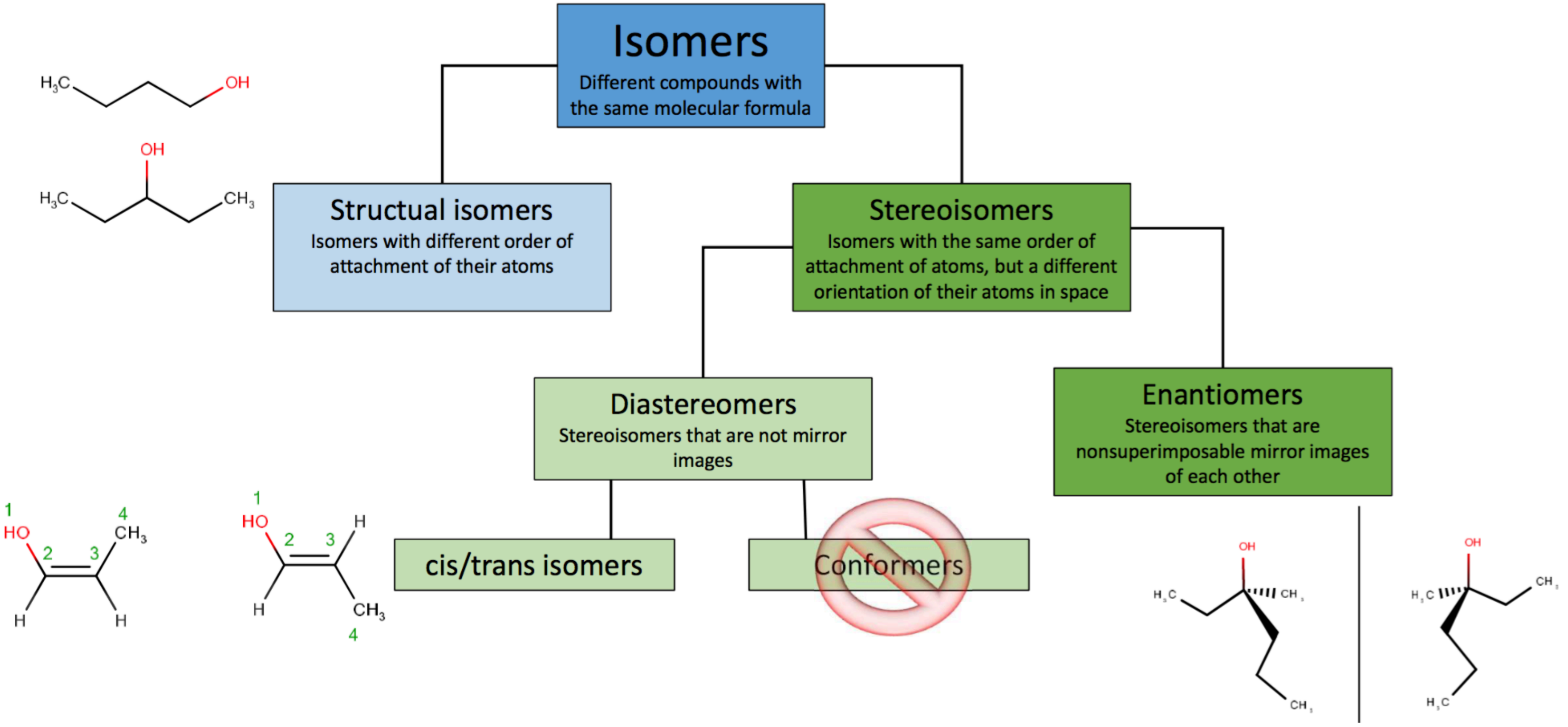
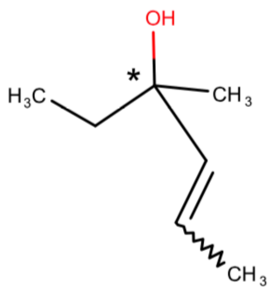
Map of Isomers

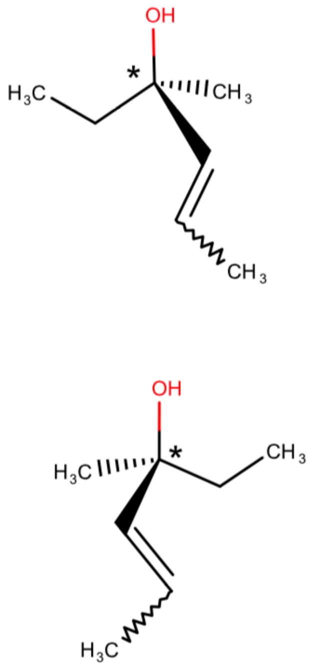


Different Classes of Stereoisomers

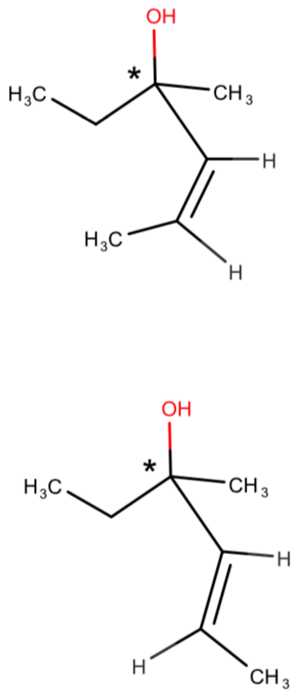
No stereo



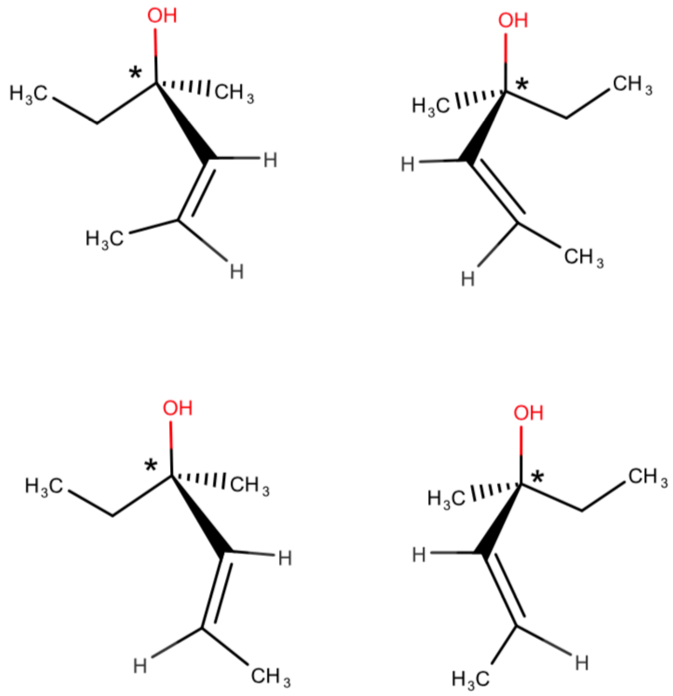
Tetrahedral Stereoisomers



Double bond Stereoisomers

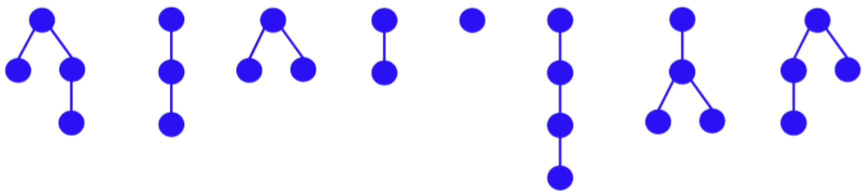


Both Tetrahedral and Double Bond stereoisomers



Molecules as Trees

T



zzzz	zzz	zzz	zz	z	zzzz	zzzz	zzzz
$+z^4$	$+z^3$	$+z^3$	$+z^2$	$+z$	$+z^4$	$+z^4$	$+z^4$

$T(z)=$ $z + z^2 + 2z^3 + 4z^4$

u		u				u	u
$+u$	$+0$	$+u$	$+0$	$+0$	$+0$	$+u$	$+u$

$T(u)=$ $4u$

zzzzu	zzz	zzzu	zz	z	zzzz	zzzzu	zzzzu
$+z^4u$	$+z^3$	$+z^3u$	$+z^2$	$+z$	$+z^4$	$+z^4u$	$+z^4u$

$T(z,u)=$ $z + z^2 + z^3 + z^3u + 3z^4u + z^4$

Iterative Method

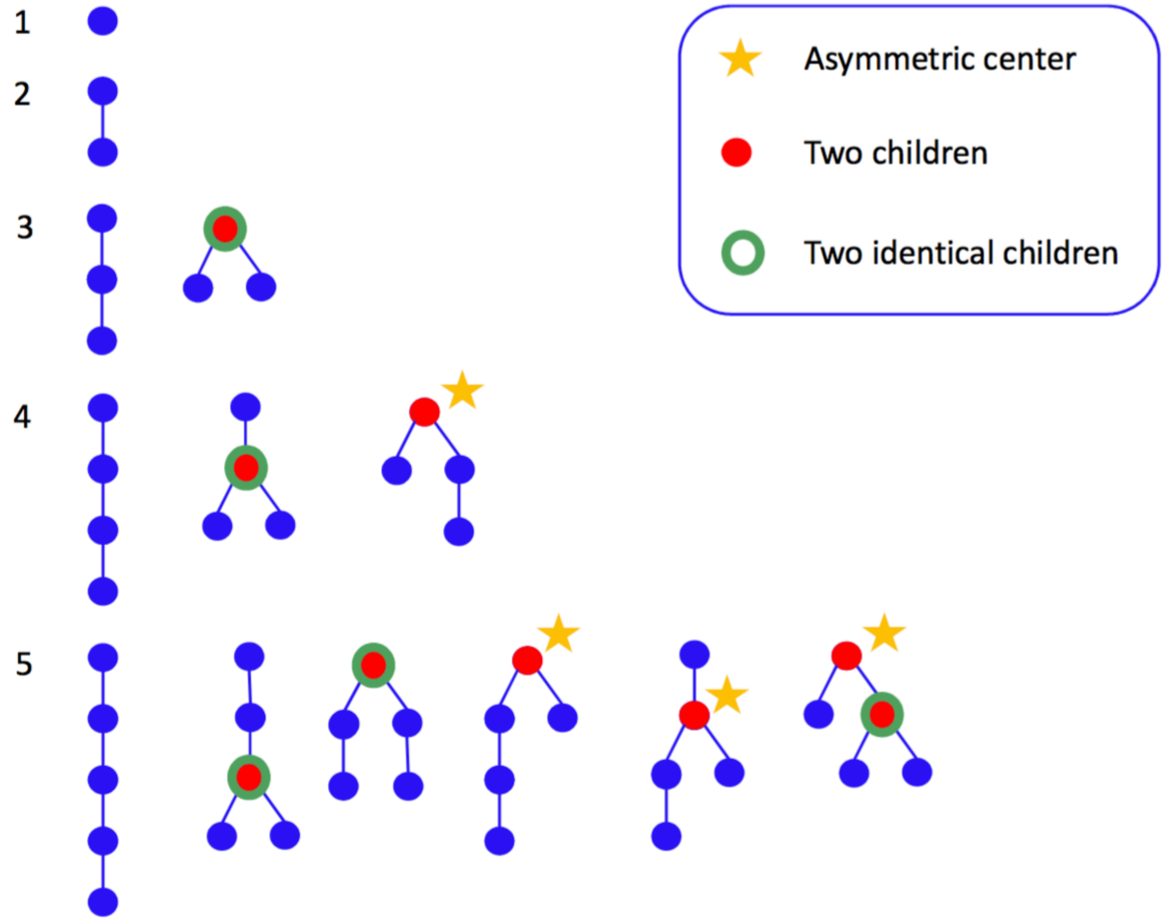
$$Y = z + z \cdot Y^2$$

$$
\begin{aligned}
Y_0(z) &= 0 \\
Y_1(z) &= z + z \cdot Y_0^2(z) \\
&= z + z \cdot 0 \\
&= z \\
Y_2(z) &= z + z \cdot Y_1^2(z) \\
&= z + z \cdot z^2 \\
&= z + z^3 \\
Y_3(z) &= z + Y_3^2(z) \\
&= z + z \cdot (z + z^3)^2 \\
&= z + z \cdot (z^2 + z^6 + 2 \cdot 2z^4) \\
&= z + z^3 + 2z^5 + z^7 \\
Y_4(z) &= z + z^3 + 2z^5 + 5z^7 + 6z^9 + 6z^{11} + 4z^{13} + z^{15} \\
Y_5(z) &= z + z^3 + 2z^5 + 5z^7 + 14z^9 + 26z^{11} + 44z^{13} + 69z^{15}
\end{aligned}
$$

$$Y(z) = z + z^3 + 2z^5 + 5z^7 + 14z^9 + 42z^{11} + 132z^{13} + 429z^{15} + ..$$

Counting Asymmetric Centers (MSET2)

$$T = Z + Z \times T + Z \times u\mathrm{MSET}_2(T)$$



$$z + z^2 + (u+1)z^3 + (2u+1)\,z^4 + \left(u^2 + 4u + 1\right)z^5$$

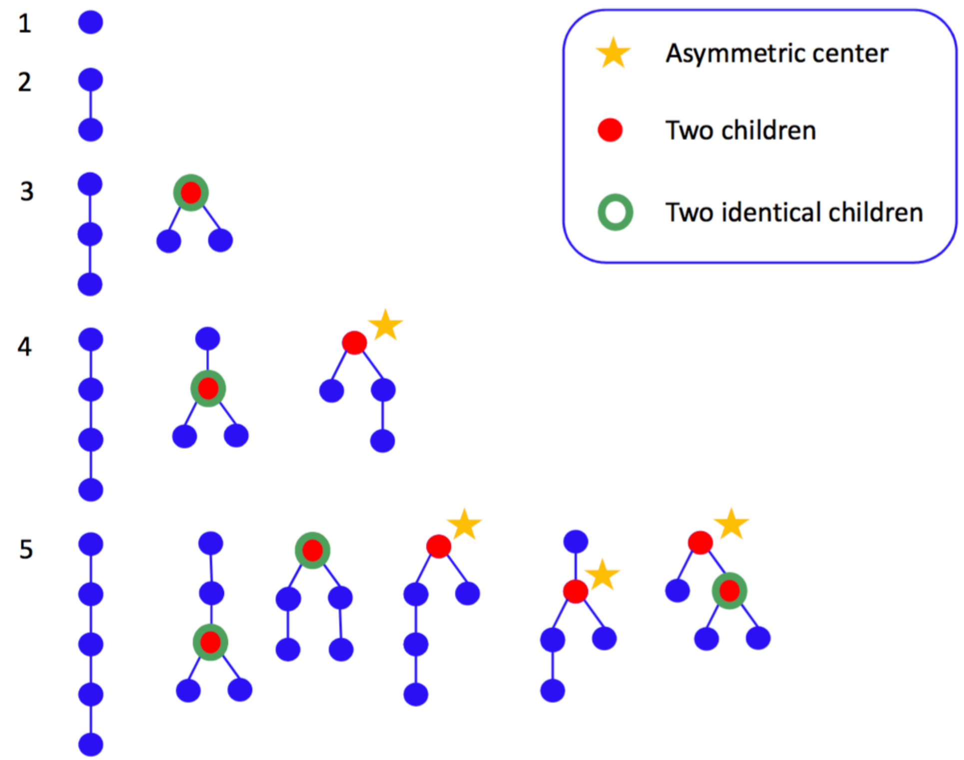
Counting Asymmetric Centers (identical children)

$$T(z) = z + z \cdot T(z)^2 + z \cdot \frac{1}{2}T(z)^2 + u \cdot z \cdot T(z^2) - z \cdot \frac{1}{2}T(z^2)$$

$$z + z^2 + (u+1)\,z^3 + (u+2)\,z^4 + (3u+3)\,z^5$$

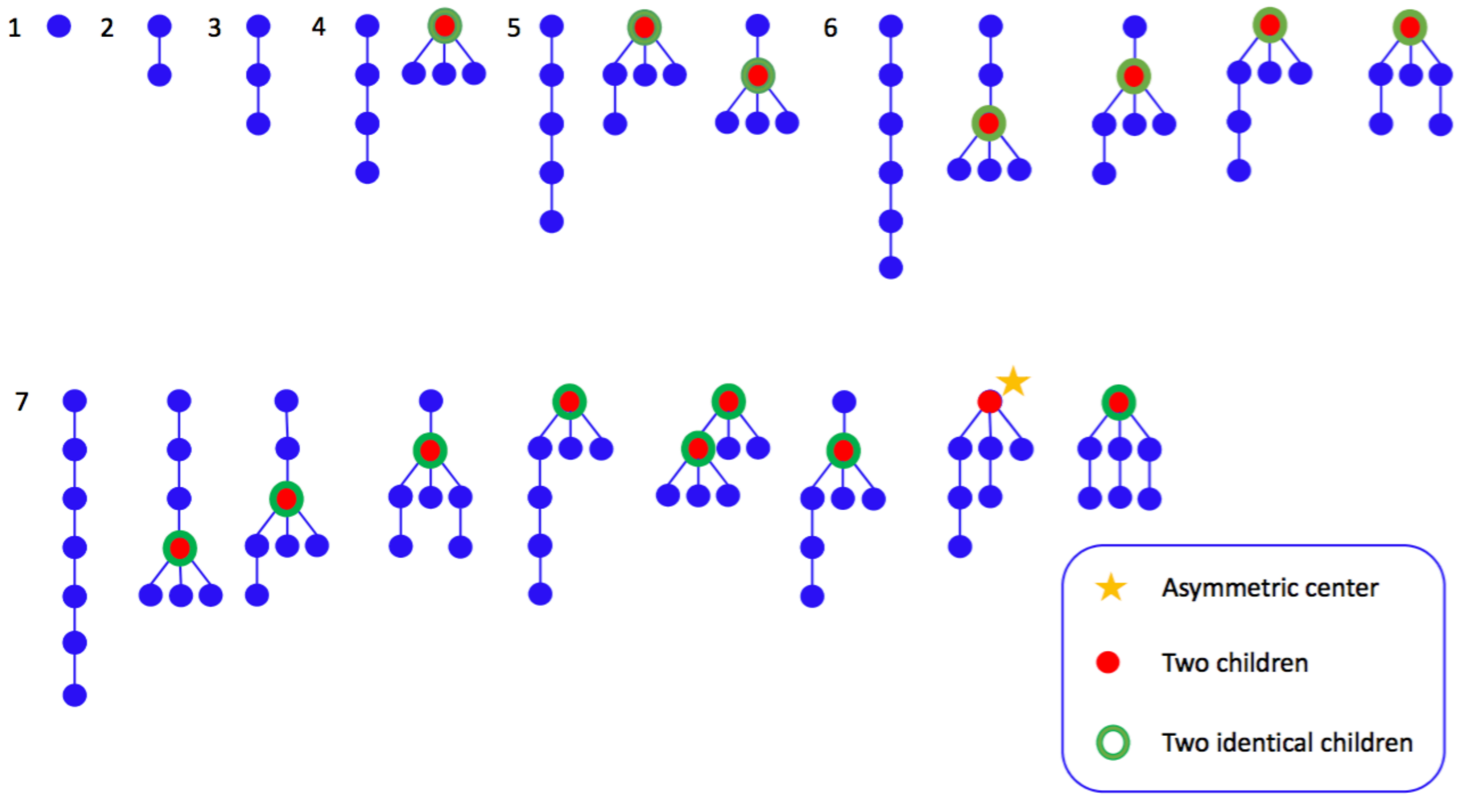
Asymmetric (all children different):

(all MSET2) – (all with identical children)



Counting Asymmetric Centers (MSET3)

$$T(z) = z + z \cdot T(z) + z \cdot \mathrm{MSET}_3(T)$$



$$T(z) = z + zT(z) + \boxed{uz\frac{1}{6}T(z)^3 + uz\frac{1}{3}T(z^3) + uzT(z)T(z^2) - uz\frac{1}{2}T(z)T(z^2)}$$

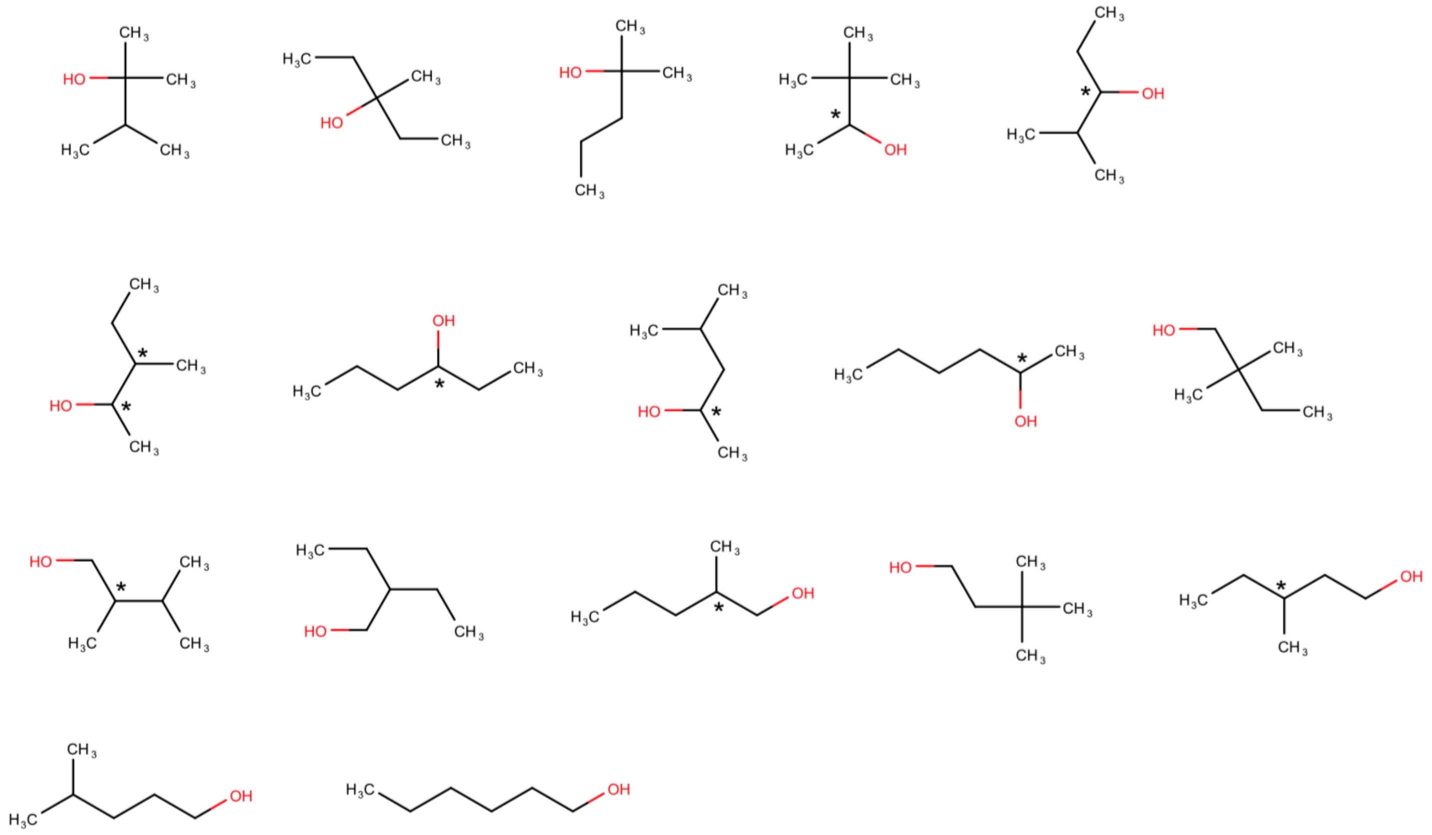
$$T(z) = z + zT(z) + \boxed{z\frac{1}{6}T(z)^3 + z\frac{1}{3}T(z^3) + uzT(z)T(z^2) - z\frac{1}{2}T(z)T(z^2)}$$

$$T(z) = z + zT(z) + \boxed{uz\frac{1}{6}T(z)^3 + uz\frac{1}{3}T(z^3) + zT(z)T(z^2) - uz\frac{1}{2}T(z)T(z^2)}$$

$$G = z + Z \times G + MSET_2(G) + MSET_3(G)$$

$$z + z^2 + 2z^3 + (u+3)\,z^4 + (3u+5)\,z^5 + \left(u^2 + 8u + 8\right) z^6 + \left(5u^2 + 20u + 14\right) z^7$$

Asymmetric Centers marked with a star



A more complex example (cis/trans + tetrahedral)