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## How to assign r and s

To name the enantiomers of a clear compound, their name must include the handedness of the molecules. This method is officially called R/S. The method of clearly assigned the handy of molecules originating from three chemistry: R.S. Cahn, C. Ingold, and V. Prelog and, as such, is also commonly referred to as the Cahn-Ingold-Prelog rule. In addition to the Cahn-Ingold system, there are two ways to determine the absolute configuration of an enantiomer: X-ray diffraction analysis. However, for non-laboratory purposes, it is beneficial to focus on the R/S system, this is because the optical rotation marker for a particular enantiomer may change as the temperature changes. The right and left hand nomi names are used to name the enantiomers of a chiral compound. The floating audio center is labeled as R or S. Consider the image first: a curved arrow is drawn from the highest priority (1) replacing the lowest priority (4) instead. If the arrow points counterclockwise (left when leaving the 12-hour clock position), the configuration in the center of the body is considered S (Sinister → Latin = left). However, if the arrow points clockwise, (Right when leaving the clock position 12 o'clock) then the floating audio center is labeled R (Rectus → Latin = right). R or S is then added as a prefix, in parentheses, to the name of the interested enantiomer. Example 1 (R)-2-Bromobutane (S)-2,3-Dihydroxypropanal Before applying the R and S to a center of chirality, the molecule must be prioritized according to the following rules: First, check at the atoms directly attached to the chiral center of the compound. An alternative to some higher atoms would be preferred over an alternative to some lower atoms. Hydrogen is the lowest possible preferred substitute, because it has the lowest atomic number. When dealing with isotopes, atoms with higher atomic masses receive higher priority. When envisioning molecules, the lowest priority alternative should always point away from the viewer (a dashed line indicates this). To understand how it works or looks, imagine that a watch and a pole. Attach a pole to the back of the watch, so that when looking at the watch face, the pole indicates away from the viewer in the same way that the lowest priority alternative will show. Then draw an arrow from the highest priority atom to the 2nd highest priority atom to the 3rd priority atom priority atoms. Because the 4th highest priority atom is placed at the back, the arrow will appear as if it were passing through the clock face. If it goes clockwise, then it is an R-enantiomer; if it goes counterclockwise, it is an S-enantiomer. When looking at a problem with wedges and dashes, if the lowest priority atom is not on the dissipated line just away, the molecules must be rotated. Remember that Wedges indicates that comes for the viewer. Dash indicates pointing out to the viewer. If there are two replacements with equal rankings, proceed along the two replacement strings until there is a difference. First, determine which chain has the first connection to an atom with the highest priority (the highest number of atoms). That chain has a higher priority. If the strings are similar, proceed down the string, until a difference. For example, an ethyl alternative has priority over a methyl substitute. At the stereocenter's connection, both have a carbon atom, which is equal in rank. Going down the chains, a methyl has only hydrogen atoms attached to it, while ethyl has another carbon atom. Carbon atoms on ethyl are the first difference and have higher atomic numbers than hydrogen; therefore ethyl is preferred over methyl. If a chain is connected to the same type of atom two or three times, check that the atom it is connected to has a larger atomic number than any atom to which the competing chain is connected. If no atom is connected to competing chain(s) at the same point with a larger atomic number: the chain associated with the same atom multiple times has a greater priority. If however, one of the atoms connected to the competing chain has a higher atomic number: that chain has a higher priority. Example 2 A 1-methylethyl alternative is preferred over an ethyl alternative. Connected to the first carbon atom, ethyl has only one other carbon, while 1-methylethyl has two carbon atoms attached to the first atom; This is the first difference. Therefore, 1-methylethyl ranks higher in preference than ethyl, as shown below. However: Remember that being doubled or tripled linked to an atom means that the atom is connected to the same atom twice. In this case, follow the same method as above. Caution! Keep in mind that priority is determined by the first spread along two similar alternative chains. After the first difference, the rest of the string is inappropriate. When looking for the first point of difference on the same alternative string, one may encounter branching. If there is a branch, select a branch with a higher priority. If two substituents have similar branches, rank the elements in the branches until a difference. After all your replacements have been prioritized correctly Now you can name/label molecules R or S. Put the lowest alternative priority at the back (dissipate the line). Conduct from 1 to 2 to 3. (It is useful to draw or imagine an arcing arrow that goes from 1 → 2 → 3) Determine whether the direction is 1 to 2 to 3 clockwise or counterclockwise. i) If it is clockwise it is R, ii) if it is counterclockwise it is S. USE YOUR MODEL KIT: The model assists in visualizing the structure. When using a model, make sure the lowest priority is heading away from you. Then determine the direction from the highest priority alternative to the lowest: clockwise (R) or counterclockwise (S). IF YOU DON'T HAVE A MODEL KIT: remember that the dash means the bond is going to the screen and wedges mean the bond is coming off the screen. If the lowest priority bond is not pointed to the back, the spiral rotates it so that it is. However, it is useful when learning organic chemistry to use models. If you have a model set use it to help you solve the following practice issues. What is the following R or S? Solution S: 1 → 2 → 3: F → G → H. The lowest priority substituent, H, was going backwards. It turns left going from 1 to 2 to 3, so it is an S. R: Br → Cl → CH3 → H. The lowest priority, at the back. Then go from Br to Cl to CH3 is turning right, giving you an R. Both R or S: This molecule is achiral. Only chiral molecules can be named R or S. R: OH → CN → CH2NH2 → H. H, the lowest priority, must be switched to the rear. Then, going from OH to SUN to CH2NH2, you're turning right, giving you R. (S) S: (Ce(-COOH)) → (Ce(-CH, 2OH)) → (Ce(C#CH)) → (Ce(H)). Then go from (Ce(-COOH)) to (Ce(-CH, 2OH)) to (Ce(-C#CH)) you're turning left, giving you to configure S. Schore and Vollhardt references. Organic chemical structure and function. New York: W.H. Freeman and Company, 2007. McMurry, John and Simanek, Eric. The basic principle of organic chemistry. Ed. Brooks Cole, 2006. Contributors Ekta Patel (UCD), Ifemayowa Aworanti (University of Maryland Baltimore County) Chiral centers have two flavors - vanilla or chocolate chips... Just kidding! They come in R and S varieties. There is a three-step process for assigning R or S and one of the steps in placing the lowest priority group behind you. But what do you do when the lowest priority group doesn't behave and isn't yet behind? Read on and watch the video to figure out two simple strategies that will shake your chiral world! More... What happens when hydrogen doesn't work? In the video below, I briefly summarize the rules for assigning R and S. However, the focus of the video is on two rule-based approaches to assigning the absolute configuration of a chiral center when the lowest priority group does not behave and is not yet in its usually a hydrogen - you know you can't trust these little rascals! An R and S configuration trick? I hate to say anything is a trick, but if this works for you, then call it what you will! ☺ Good luck, and let me know how you're going with R and S in the comments below! If we name these two alkyl halides based on the IUPAC nomi names, we get the name 2-chlorobutane for both: However, they are not the same compound - they are enantiomers: So we need to add a piece of information to distinguish the enantiomers (and other isologues) by their names. Cahn, Ingold, and Prelog have developed a system that, regardless of the direction we are looking at molecules, will always put the same name (unlike wedge marks and dashes). And that's why this is also known as absolute configuration or commonly known as system R and S. Let's see how it works by looking at the following molecules and we'll go back to 2-chlorobutane then: Assign R and S configurations: Steps and rules To assign absolute configuration, we first need to locate carbon(s) with four different groups (atoms) connected to it. They are called chirality centers .... In our molecules, we only have one carbon with four different groups and that is one with bromine and we will specify the absolute configuration of this chiral center. For this, you need to follow the steps and rules of the Cahn-Ingold-Prelog system. Step 1: Give each atom connected to the chiral center a priority based on its atomic number. The higher the number of atoms, the higher the priority. So based on this, bromine is given one priority, oxygen is preferred two, carbon methyl is third and hydrogen is the lowest priority-four: Step 2: Draw an arrow starting from priority one and go to priority two and then prioritize 3: If the arrow goes clockwise, just like in this case, the absolute configuration is R. As opposed to this, if the arrow goes counterclockwise then the absolute configuration is S. As for example, in the following molecules, the priorities go Cl → N → C → H and the counterclockwise direction of the arrow indicates an absolute configuration S: So remember: Clockwise - R. Counterclockwise - S. Now, let's see what will be the absolute configuration of enantiomer: The priorities remain the same because all groups around carbon are the same. Starting at Bromine and going to oxygen and then carbon, we can see that this time the arrow goes counterclockwise. If the arrow goes counterclockwise, the absolute configuration is S. And this is an important thing to remember: All the chirality centers in the enantiomers are reversed (each R is S, each S is R in enantiomer). So we discussed the role of priorities 1, 2 and 3 but what We didn't mention anything about the arrow that goes to it. It is part of the game and how do you use it? The lowest priority does not affect the arrow orientation. However, this is very important, and it is a requirement when assigning configurations R and S, that: The lowest priority must be away from the viewer. In other words, the lowest priority must be a dashed line to assign R and S based on the direction of the arrow as we just did: With that in mind, how can we assign the absolute configuration of this molecular, where hydrogen is a wedge line towards us? R and S When the lowest priority is a wedge You have two options here: Option one. Rotate the 180° molecular so that hydroxyl is now facing you and hydrogen is just going. This allows to have molecules drawn as needed, prioritizing the lowest backward pointing as it is supposed to be to define configuration R and S: Next, specify priorities: chlorine-number one, oxygen-two, carbon-three and H are number four. The arrow goes clockwise, so the absolute configuration is R. The problem with this approach is that sometimes you will work with larger molecules and it is not practical to redraw entire molecules and exchange each single chirality center. For example, look at biotin with all hydrogens pointing forward. Not the best option to redraw this molecular change all hydrogen and keep the rest of the molecules as it should be. This is why we take the second approach that's what people usually follow. Here, you leave the molecules as it is with hydrogen pointing towards you. Continue as you usually do by assigning priorities and drawing arrows. The only thing you have to do at the end is change the result from R to S or from S to R. In this case, the arrow goes counterclockwise but because hydrogen is facing us, we change the result from S to R. Of course, either approach should give the same result because this is the same differently drawn molecule. R and S When group #4 is not a Wedge or Dash There is a third possibility for group 4's position and that's when it isn't just going or on your side. This means we can't define the configuration as easily as if the lowest priority is heading towards or away from us, and then turning it to the end as we did when group 4 was a wedge line. For example, what is the configuration of this molecular? For this, there is such a simple but useful trick that makes life much easier. Remember: Exchange any two groups on a chiral center that reverses its absolute configuration (R to S, S to R): Notice that these are different molecules. Let's not talk about rotating about a single axis or link, in which case the absolute configuration(s) must remain the same. We are actually converting to another Groups to make it easier to define configuration S R and S. Let's do this on the molecules mentioned above: The lowest priority group is in the drawing plane, so what we can do is swap it with molecules that are pointing away from us (Br). After determining R and S, we convert the result because the exchange means absolute configuration changes and we need to switch back again. The counterclockwise arrow indicates the S configuration, and this means that in the original molecular it is R. In addition, it takes more time, you can draw the Newman projection of the visible molecules from the angle of placing group 4 at the back (pointing out the viewer): The lowest priority group is pointing and therefore, clockwise direction of the arrow indicates the configuration R. R and S when the atom (group) is the same Sometimes it happens that two or more atoms connected to the chiral center are the same and it cannot specify immediate priorities. For example, let's go back to 2-chlorobutane starting with clenbutane: Chlorine is the top priority, then we have the two lowest priority carbon and hydrogen. We need to determine the second priority of comparing two carbon atoms and having a tie since both (obviously) have the same number of atoms. What do you do? You need to look at the atoms connected to those you compare: The left carbon (CH3) is connected to three hydrogen, while the right one is connected to two hydrogen and one carbon. This additional carbon second priority for CH2 and CH3 is prioritized three. The arrow goes clockwise, so this is (R)-2-chlorobutane. And if these atoms are also identical, we will have to move further from the chiral center and repeat this process until we reach the point of difference first. It's like layers: the first layers are atoms connected to the chiral center, and you're comparing them and only moving to the second one if there's a tie. You should never compare any atom of the second layer with a first-class atom regardless of its atomic number. Double and triple bonds in configurations R and S Make R and S for this molecular: Bromine is the priority and hydrogen is number four. Carbon a is connected to one oxygen and two hydrogen. Carbon b is connected to an oxygen and a hydrogen. However, due to the double bonds, carbon b is considered if it is connected to two oxygen. The same rule applies to any other double or triple link. So when you see a double bond count it as two single bonds when you see a triple bond cut it as three single bonds. The arrow goes clockwise, however, the absolute configuration is S, because hydrogen is heading towards us. More tricks in configuring R and S What if you are comparing two carbons: one connection with three high atomic numbers and the other one with two hydrogen and one heteroatom. Which one gets higher priority? Take a look at this with this module: Even if only one atom has a higher atomic number than the highest number of other carbon atoms, the group will take precedence. So an S beats N, O, F because it has some atoms higher than others individually. Carbon is not the only atom indicated by R and S. In theory, any atom with four different groups is chiral and can be described by the R and S systems. A pair of smaller solitary electrons. Carbanions are achiral because solitary pairs quickly flip from side to side unless at very low temperatures: R and S do not apply to nitrogen in amines for the same reason as for carbanions. However, second-order ammonium groups may be chiral. The same factors can receive different priorities based on its iso isotho. For example, atomic tritium has a higher priority deuterium: T → D → H: You can practice these rules to assign R and S configurations on this page: R and S configuration practice problems Check Also in Stereochemistry: Take Now

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