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Constraint vs restraint

According to the norm, it is difficult to live in many aspects of human life without restrictions. Despite the fact that no one likes these restrictions, they are sometimes unavoidable and set limits in many things. Restrictions can be set by a person, the law, or the human instinct. Restriction and restraint are two words that show different types of constraints and, although interchangeably used, are very different. What is restriction? A constraint is a restriction or restriction for someone or something. It is also used in a situation where there is discomfort between two people regarding their relationships. Restrictions are triggered by their own internal and deep-rooted standards and values. A person may be subject to political, temporal, legal, economic and financial constraints, to name but a few. For example, time can be a constraint factor to complete some work. It can also be used in a scene that shows the level of restraint in relationships between people. An example in a sentence that explains this would be that, after such a long time, I spoke to him without coercion. What is restraint? Reticence is the act of restraint. It may also refer to the action to keep something or someone under control, moderate behavior or self-control, a device used for restraint, and the restriction of freedom of movement or personal freedom. Both relate to restrictions that impose constraints on people and things differences between coercion and restraint, while a restriction is a restriction or restriction for someone or something, a restraint is an act of holding back or holding something or someone under control. While restrictions are triggered by their own internal and deep-rooted standards and values, restrictions are caused by both individuals and other people. One example is the law's restrictions on certain activities. A constraint is more often a situation or problem. For example, a financial constraint is a problem. On the other hand, restraint refers to a restriction of an act or an individual. For example, the court may issue an injunction against an individual. Restriction vs. Restraint: Comparison Table Summary of Restriction vs. Restraint It is important to understand the use of words constraints and constraints. While the word restriction is used to prevent someone from taking a specific action a reluctance is an act of keeping something or someone under control. Tabitha graduated from Jomo Kenyatta University of Agriculture and Technology with a bachelor's degree in commerce, specializing in finance. She had the pleasure of working with various organizations and gained expertise in business administration, business administration, accounting, finance and digital marketing. The true power of the atomistic description of a molecule embodied in energy expression lies in two main areas. The first is Analysis of energy contributions at the level of each or class of terms. For example, you can decompose the energy in binding energies, angular energies, non-bound energies, etc., or even to the level of a particular hydrogen bond or van der Waal's contact to understand a physical observable or make a prediction. The second area described in the following sections is to change the energy expression to distort the calculation. You can set constraints (absolute conditions), such as.B to fix an atom in space and not to allow it to move. You can also add additional terms to the energy expression to restrict or enforce the system in a certain way. For example, if you add an additional torsional potential to a particular binding, you can force the torsion angle toward the desired value. The crucial difference between a constraint and a restriction is that a constraint is an absolute limitation imposed on the calculation, while a constraint is an energetic distortion that tends to force the calculation towards a particular constraint. Restrictions and constraints allow you to focus the calculation on a region or conformation of interests, and also to set up computational experiments. Such experiments are one of the primary applications of molecular modeling, so you can control a molecule - or at least the model of the molecule - at the atomic level. Fixed atomic restrictions Solid atoms are limited to a certain position in space, they cannot move at all. Solid atoms reduce the cost of a calculation in two ways. First, terms in energy expression that only affect solid atoms can be eliminated because they add only one constant to the total energy. Since the positions of fixed atoms cannot change, the contribution of terms that depend only on these positions cannot change. Second, fixing atoms reduces the number of degrees of freedom in the system, allowing minimizers to converge in fewer steps, and the dynamics require fewer steps to sweep out the available conformation space. Note that the energy calculated by the Discover program applies only to any constant, depending on the molecule and the solid atoms. Therefore, only differences in energy between denconations of the same molecule with the same solid atoms are useful. Distance restrictions Distance restrictions are used to force the distance between two atoms, bound or not, to a specific value. The Discover program supports two most commonly used functional forms. One is a simple harmonic function: Eq. 2-15: where K is a force constant, Rij is the current distance between the atoms and Rtarget the target distance. A large force constant tends to force the distance near the target distance; a smaller force constant results in a correspondingly smaller distortion. The second form is also a harmonic potential, but it is divided into five piecemeal continuous areas: Eq. Eq. This flat potential is illustrated in Figure 2-12. Note that the potential does not have to be symmetric and that after the appropriate definition of points R1, R2, R3 and R4, one of the regions can be eliminated. The important areas are those from R1 to R2 and from R3 to R4, where a harmonious potential is applied, and the flat soil from R2 to R3. This form of restraint allows for a number of acceptable distances and is particularly useful for including experimental distance information in a calculation. The flat floor allows an experimental error in the determined distance. The two outer regions have a constant gradient, which is useful for avoiding ridiculously large forces when the original structure is far from the target value. Torsion restrictions As distance restrictions, different forms of torsional restrictions are used in literature. These range from a simple harmonic form analogous to Eq. 2-15 to the piecemeal continuous form of Eq. 2-16 with R interpreted as an angle instead of distance. Another natural form is the periodic function of Eq. 2-17: Eq. 2-17: where V is the strength of the restraint, n is an integer periodicity and 0 is the phase angle. The harmonic restraints or those of Eq. 2-17 with n = 1 are suitable to force a torsion angle to a certain value. The periodic form with a periodicity greater than one is useful for limiting a torsion to one of several related angles. A triple potential could hold a torsion either trans or at one of the two Gauche conformations.B, depending on the initial conformation and the strength of the used potential. Template Forcing To force the conformation of a molecule to be similar to that of a stencil molecule, one of the following restriction terms for energy expression is added: Eq. 2-18: or: Eq. 2-19: The term in Eq. 2-18 is proportional to the root-middle-square deviation of the analog atoms from the schablonatom. Eq. 2-19 represents a conceptually simpler restraint, whereby each analog atom is introduced by an isotropic spring to the position of its stencil atom. In both forms, the sum is above a list of atomic pairs that are supposed to hold back: one from the moving analogue and one from the template molecule. The first form gives the best rms fit for the lowest energy cost, but individual atoms can stay quite far from their template position. The second form holds each atom back individually, forcing each atom to its template partner. The resulting rms fit is not as good as Eq's. 2-18, but no atom may be as far as possible with Eq. Differ. The shape in Eq. 2-19 also allows a different force constant for each pair, which means that different atoms or atomic classes can be treated differently. Tethering Tethering is a special case of template enforcement. The atoms are to their original positions and not to the positions in a template structure. Both Eq. 2-18 as well as Eq. 2-19 are applicable for tethering, although Eq. 2-19 is usually preferred, since tethering is usually used to prevent atoms from moving too far from their original positions. Main access page Theory/Methodology Access. Describe-System Access Ewald Sums Forcefields Copyright Biosym/MSI What is the difference between 'Constrain' and 'restrain'? Restricting and withholding are two words that are very similar and often abused because their definitions have similarities that appear minor but differ greatly in practice. CONSTRAIN refers to something that prevents you from doing something. Helga was limited by her duty to her family. The constraints of the law kept Fergal from killing every stupid person in the room, even though he really wanted it. RESTRAIN refers to something that prevents you from doing something. I had to be restrained when I went to the Hershey store. So. Lots. Chocolate. Fergal gave in to temptation and had to be restrained before his frustration led to him killing the stupid people outside the room. Remember to limit as a fence that keeps you in and inhibits you, but you can jump over it if you really want (and then deal with the consequences). Restrain is like a rope that binds you and keeps you from jumping anything unless you're a character in Fifty Shades of Grey. I felt the CONSTRAINTS of a humble company that broke against my bare flesh as I walked naked through the supermarket before the security guard decided to call me and the police.

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