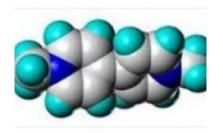
## What Is Paraquat And How Bad Is It?



(/profile/josh-bloom) By Josh Bloom (/profile/josh-bloom) — December 22, 2016

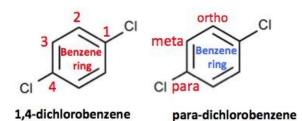


Paraquat Molecular Model Source: Paraquat.com

Although the name paraquat may sound like a chimeric entity derived from combining the DNA of parakeets and wombats, or those of you who happened to be alive, it is simple, but notorious (1) herbicide. And its name even makes sense.

$$H_3C-N$$
 $N-CH_3$ 
 $CI^-$ 

The chemical structure of paraguat



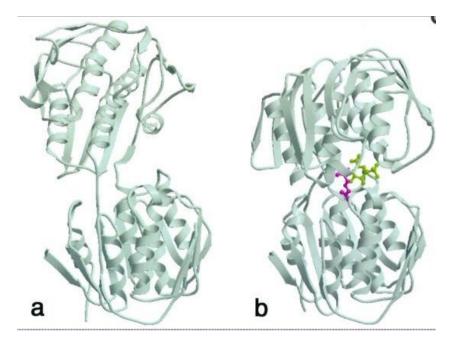
(these are identical)

The term "para" refers to the relative position of two atoms (aside from hydrogen) on a benzene ring (and other common rings as well). Para means that the two groups are as far away as possible across the ring from atom 1. (The name 1,4dichlorobenzene can be used interchangeably with para-dichlorobenzene.) Meta (1,3) is the next closest, and ortho (1,2) is the closest. Paraguat has two prominent examples of para substitution.

The other part of the name also makes sense—a rarity in the world of organic chemistry. Amines, which are derivatives of ammonium bearing either one, two, or three carbon atoms, have the unique ability to accept a fourth carbon, in the example below, methyl. Once this group is added, it is now called a quaternary salt. Para. Quat. There you go.

Paraquat is in the news because of toxicity concerns, discussed in an article (http://www.nytimes.com/2016/12/20/business/paraquat-weed-killer-pesticide.html?\_r=0) in the December 20th *New York Times,* so this is a good time to examine what paraquat does and doesn't do.

Ideally, a pesticide or herbicide (and "cide," really) should target the pest by disrupting a process that does not have a human counterpart. For example, glyphosate shuts down one of seven biochemical steps in the shikemic acid pathway in plants by inhibiting an enzyme called 5-enolpyruvylshikimate 3-phosphate synthase. This, in turn, prevents the plant from biosynthesizing three essential acids, so the plant cannot grow.



Ribbon diagram of 5-enolpyruvylshikimate 3-phosphate synthase. The structure on the left is the enzyme alone. On the right, the enzyme is bound to glyphosate. Note how glyphosate occupies the active site (where the reaction takes place) of the enzyme and also changes its shape. Image: PNAS

But, humans (all animals, really) do not have (or need) 5-enolpyruvylshikimate 3-phosphate synthase, so there is nothing for glyphosate to inhibit. This is exemplified (table below) by comparing the relative  $LD_{50}(2)$  values of glyphosate to common substances.

Chemical Glyphosate	Toxicity relative to glyphosate	
	1.0	Least toxic
Salt	1.4	
Vitamin A	2.5	
Tylenol	2.6	
Aspirin*	3.1	
Arsenic (metal)	6.6	
Caffeine	14.9	Most toxic
Morphine	35.7	
* Female rats		

Relative toxicity of some common chemicals. Source: Sigma-Aldrich safety data sheets.

But the situation is entirely different for paraquat. Paraquat is toxic. Its relative toxicity to glyphosate ranges from 33-250. A lethal dose in average person is about 2.5 grams, and it is even more toxic when inhaled. So, what is going on here?

Next: Part 2- The real risk from paraquat. How bad is it really?

## Note:

- (1) For those of you unfortunate enough to be old, you may remember a big stink in the 1980s when the DEA used it to try to eradicate homegrown marijuana (http://www.nytimes.com/1988/07/14/us/us-to-resume-using-paraquat-on-marijuana.html). This didn't go over too well.
- (2) The  $LD_{50}$  is the dose of a particular chemical that will kill half of the test animals. It is usually determined by a single oral dose.