

# Beyond the Printed Page

## Élan Tool Bar

## Get Started Fast

Click the special Élan button in Microsoft Word, and Élan automatically creates a notebook page for you. From there, simply draw a reaction in ISIS/Draw or build on past work by conducting any number of sophisticated searches. You can retrieve, for instance, information about all experiments performed on a given day, or experiments involving a particular chemical reaction. Once you've copied any pertinent information into your new notebook entry, Élan automatically calculates molecular weights and molecular formulas for the reactants and products and provides space for you to enter information about the apparatus.



## Provide Protocols and Vital Context

Élan gives you all the space you need to document synthetic procedures. Protocols stored in Élan can be easily reused by colleagues in conducting their own experiments and pasted into materials and methods sections of papers should you decide to publish your work.

## Collect Analytical Data

You can collect analytical results in this table and even track the status of tests. Visual indicators make it easy to see where things stand—the envelope icon, for instance, indicates that tests have been requested.

Élan can even generate an analytical sample submission form, completely filled in based on the information in your notebook entry.



Projects

ELAN\_Lab1\_HC\_1\_002 - Microsoft Word

Élan Edit View Insert Format Tools Tables Window Help

Henry Christian

Experiments Data Tables Calouts

**Synthesis of 2,6-Dichloro-9-thiabicyclo[3.3.1]nonane**

Electrophilic scaffolds Project No. 4242

Electrophilic addition Step 1

HC-0001-001

108.18 C<sub>8</sub>H<sub>14</sub>

211.15 C<sub>8</sub>H<sub>10</sub>Cl<sub>2</sub>S

91.9 %

Apparatus: 200 ml 3-neck flask equipped with a Teflon-coated magnetic stir bar, a 25-ml pressure-compensating addition funnel with nitrogen inlet, thermometer, and standard taper stopper. Heated entire apparatus under dry nitrogen flow to remove all visible water.

amt	unit	mmol	equiv	description
100.0	g	905.9		1,5-cyclooctadiene (Fluka - 29598, 98 %)
94.70	g	905.9	1.00	Sulfur dichloride (074665_DJ_3_134, 98.5 %)
600	ml			Hexane (Fluka 52765)

A 200 ml 3-neck flask was equipped with a Teflon-coated magnetic stir bar, a 25-ml pressure-compensating addition funnel with nitrogen inlet, thermometer, and standard taper stopper. The stopper was removed and dry nitrogen was flowed through the apparatus while heating all glass surfaces with a heat-gun until all visible water condensation was driven from the surfaces. The nitrogen flow was then switched from "flow" to "vent" and the stopper was replaced. After the apparatus was cool, the flask was charged with the sulfur dichloride and 80 ml of dry hexane, and the flask was immersed in a dry-ice/acetone bath. The cyclooctadiene was then charged to the addition funnel. The magnetic stirrer was raised, and the cyclooctadiene was added dropwise, to keep the reaction temperature below -40 deg C. After the addition of cyclooctadiene was complete, the addition funnel was rinsed with ca. 10ml of additional dry hexane; this was added to the reaction mixture. The dry-ice/acetone bath was removed, and the mixture allowed to come to room temperature.

TLC of the warmed reaction mixture showed a nearly quantitative conversion of the 1,5-cyclooctadiene. The product crystallized directly from the reaction mixture. The reaction mixture was filtered, and the resulting white, fluffy crystals were recrystallized from fresh, dry hexane.

product	amount	unit	purity	physical properties	100% amt.	yield
1 (211.15)	177.6	g	99	m.p. = 33-36°C	191.3 g	91.9 %

final analytics	NMR	IR	MS	EA	GC/HPLC
1 (211.15)	1H-248.04	KB-248.04	MS-248.04	EA-248.04	X

comments: Very exothermic reaction; use caution at larger sizes

Reaction Specification: *quite optimized*

Title

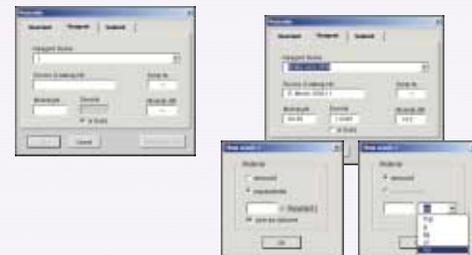
Experiment Type

Note Book Number

## Summarize Synthetic Details

When you enter a reaction or copy one into Élan, this table is automatically generated. If you have copied a reaction from a prior experiment, Élan will provide the table fully completed. For a new reaction, Élan prompts you to enter the first material.

Click "add next" and Élan will use your initial entry to determine the amounts of subsequent materials.



## Include Graphics and Annotations

Chemical structures, chromatograms, screening tables, spectra, graphs—any object that can be pasted in Microsoft Word can be included in an Élan notebook entry. And a click of a mouse lets you annotate your graphic, providing helpful context for others who might need to repeat your work in the future.

## Record Results

Using the initial synthetic details contained in the materials table, Élan generates this results table and supplies the theoretical reaction yield. Once you've completed the reaction, simply enter the amount of product isolated and its purity—a click on the blue "yield" in the results table updates the value.

## Comment on Your Work

Élan offers two ways for you to annotate and comment on your entry. The "Reaction Specification" relies on a controlled vocabulary that describes the reaction's status (e.g., an experimental technique or an optimized reaction). To provide more detail, simply type your comments in the "comments" box.