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RESEARCH ARTICLE

BIOTECHNOLOGY

X-RAY CRYSTALLOGRAPHIC STUDIES OF SYSTEMIC FUNGICIDE SULPHUR

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ABSTRACT

Plant diseases are characterized by wilting, moldy coatings, rusts, blotches, scabs and rotted tissue. They are often encouraged by wet weather, poor drainage or inadequate airflow. Some fungal problems can be controlled by reducing high moisture conditions and by cutting away diseased plant parts. In most cases however, a fungicide will be required. The organic fungicides we offer are least-toxic and earth-friendly. For best results apply early, before diseases become aggravated.` An excellent organic fungicide, Sulfur Plant Fungicide is a finely ground wettable powder containing 90% elemental sulfur, Control diseases of fruits, vegetables and flowers and effective against powdery mildew, rust, scab, brown rot, rose black spot and many more. There is large number of chemical compounds for the protection of crops available commercially in the market but their effects depends on the climate, type of soil, and other physical parameters. The interactions of proposed fungicides with the macromolecule of the parasite are dependent on the stereochemistry of these compounds. In order to design more effective synthetic fungicides, it is necessary to analysis the three dimensional structure of these compounds and if possible the receptor molecule .Recently it has been observed that some of the fungicides are loosing their effects. if their structures are known, So analogous compounds can be designed as substitute.

KEYWORDS

X-ray crystallography, Systemic fungicides, Triazole structure

INTRODUCTION

Lime-sulfur, a fungicide composed of inorganic sulfur and lime, is commonly used today to control a variety of diseases such as plum pockets, black knot, black spot of rose, and a number of raspberry diseases. Lime-sulfur was originally developed in 1851 by Grison who was the head gardener at the vegetable houses in Versailles, France. Grison boiled "flowers of Sulphur", freshly slaked lime, and water for 10 minutes, drew off the clear liquid and mixed it with water. He then used this solution to protect plants against mildews. The solution was originally known as the "Grison Liquid" or "Eau Grison". In 1886, lime-sulfur was used to control peach leaf curl in California.

Sulfur is the only ingredient in the mix that is toxic to pathogens. It is able to kill pathogens through direct contact or fumigation (sulfur vapors). The vapor action of sulfur allows the fungicide to be effective from a distance and is important in killing spores of powdery mildew. Once taken up by the fungus, sulfur disrupts the transfer of electrons causing the reduction of sulfur to hydrogen sulfide (H2S), which is toxic to most cellular proteins.

Sulfur itself is also toxic to certain plant species and is capable of causing a phytotoxic reaction. As a result, lime has been added to the mix to reduce the phytotoxicity of sulfur. The more lime added to the mix the less phytotoxic. In general, lime is considered a "softeners" for the plant.

According to the label, lime-sulfur can be applied as a dormant season fungicide or as a growing season spray. Dormant season applications need to be applied in late winter or early spring when temperatures are above freezing, but before leaves are present on the plant. Growing season applications can be made after leaves are present on the plant, but should be applied in the early morning or late afternoon to avoid burning. Plant damage caused by lime-sulfur is most severe during dry weather when temperatures reach 80 degrees to 95 degrees F. Lime-sulfur is corrosive to the eyes and harmful if swallowed, inhaled, or absorbed through the skin. Appropriate precautions according to the label should be taken when applying lime-sulfur. Thoroughly read the label before purchasing, handling, or applying lime-sulfur.

is a contact fungicide and their Symbol is S but their Chemical formula are S_8 . Atomic mass of Sulphur is equal to 32.063 *8 = 256.53.The Sulphur structure is rhombic or monoclinic nature.

Experimental procedure

Yellow well formed crystals of size *0.30 x 0.20 x 0.20 mm* are obtained by slow evaporation from a solution of Toluene and Acetone at 297□K temp within 5-7 days. These contact fungicide is soluble in water, Acetone, Toluene, and Methanol but mostly soluble in Toluene ($C_6H_5CH_3$) at temperature 20-25 degree..Table 1 shows some important properties of Sulphur

Table 1
Sulphur (Contact fungicide).

Fungicide name	*Sulphur*
Lattice types	*Rhombic or monoclinic*
Fungicide types	*Contact fungicide*
Chemical formula	*S8*
Chemical weigth	*256.53*
Physical state	*Solid*
Appearance form.	*Yellow colored lamps, Crystal, Powder*
Odor	*Odorless*
Purity	*90% - 100%*
Vapour density (Air = 1)	*1:1*
Vapour pressure	*Ommitc at 280 oF*
Boilling point	*832 oF (444 oC)*
Freezing or Melting point	*230 – 246 oF (110 - 119 oC)*
Bulk density Lump	*75 – 115 Ibs/ft3 Powder 33 – 80 Ibs/ft3*
Flash point	*405 oF (207.2 oC)*
Flamable Limit	*LEL : 3:3 VEL :46 :0*
Auto-ignition temperature	*478 – 511 oF (248 - 266 oC)*

Solubility: In water is greater than 20-25 degree C.The solubility of other Chemical solvent are :- 1. Acetone (CH_3COCH_3) 2. Toluene ($C_6H_5CH_3$) 3. H_2O and 4. Methanol (CH_3OH) etc.

Information about Sulphur (Contact fungicide)

Fungicide Name	**Use Solvent**	**Mfd Date**	**Grow time period**	**Size/shape**	**color**	**Type**
Sulphur (Contact)	Tol.+Ace+ H_2O	O8/02/11	5-7 Days	Rectangular	yellow	Single crystal

The ORTEP diagram and Packing diagram of Sulphur are solved using by SHELXS-97.The unit cell parameters a, b, and c and angle α, β and γ are determined by automatic computerized four circle Enraf- Nonius CAD-4 diffractometer.

Data collection and structure solution

The Sulphur fungicide single crystal data collection are on a computerized automatic CAD- 4 Enraf Ninius 4- circle diffractometer or Enraf Nonius CAD-4 F and CAD 4-MV31 diffractometerThe data collection is done on ω-2θ scan mode by four circl;e diffractometer.. Each intencity measurement involed in a scan over the reflection peak , a back ground measurement at each end of the scan range and measurement of peak height. The structure determination is carried out on VAX machine using SHELXS – 97.All the non hydrogen atoms are located in the beginning itself.

Refinement

The x, y and z are positional co-ordinates, which were measured from and isotropic temperature factors were subjected to refinement by SHEIXL -97 refinement computer program. After so many cycles of refinement the R dropped to 0.0316as shown in table 2.

Table 2

Cycle	(incid)	R(diffr)	Mean wt.
1	0.0473	0.0383	0.9548
2	0.0360	0.0345	0.9613
3	0.0340	0.0332	0.9622
4	0.0331	0.0326	0.9625
5	0.0327	0.0323	0.9627
6	0.0324	0.0321	0.9628
7	0.0322	0.0320	0.9628
8	0.0321	0.0319	0.9629
9	0.0320	0.0319	0.9629
10	0.0320	0.0318	0.9629
11	0.0319	0.0318	0.9629
12	0.0319	0.0318	0.9630
13	0.0319	0.0317	0.9630
14	0.0318	0.0317	0.9630
15	0.0318	0.0317	0.9630
16	0.0318	0.0317	0.9630
17	0.0318	0.0317	0.9630
18	0.0318	0.0317	0.9630
19	0.0317	0.0317	0.9630
20	0.0317	0.0317	0.9630
21	0.0317	0.0317	0.9630
22	0.0317	0.0317	0.9630
23	0.0317	0.0317	0.9630
24	0.0317	0.0317	0.9630
25	0.0317	0.0317	0.9630
26	0.0317	0.0316	0.9630
27	0.0317	0.0316	0.9630
28	0.0317	0.0316	0.9630
29	0.0317	0.0316	0.9630
30	0.0317	0.0316	0.9630
31	0.0317	0.0316	0.9630
32	0.0317	0.0316	0.9630

33	0.0317	0.0316	0.9630
34	0.0317	0.0316	0.9630
35	0.0317	0.0316	0.9630
36	0.0317	0.0316	0.9630
37	0.0317	0.0316	0.9630
38	0.0317	0.0316	0.9630
39	0.0317	0.0316	0.9630
40	0.0317	0.0316	0.9630
41	0.0317	0.0316	0.9630
42	0.0317	0.0316	0.9630
43	0.0317	0.0316	0.9630
44	0.0317	0.0316	0.9630
45	0.0317	0.0316	0.9630
46	0.0317	0.0316	0.9630
47	0.0317	0.0316	0.9630
48	0.0317	0.0316	0.9630
49	0.0316	0.0316	0.9630
50	0.0316	0.0316	0.9630

R(int) = 0.0316 (selected reflections only, after parameter refinement)

Run	2-theta	R(int)	Incid. factors	Diffr. factors	K	Total	I>2sig(I)
1	-27.0	0.0269	0.862 - 0.963	0.821 - 1.058	0.827	2103	1779
2	-24.5	0.0246	0.837 - 1.041	0.894 - 1.141	0.754	7374	6202
3	-4.5	0.0370	0.789 - 0.851	0.864 - 1.135	0.951	767	678
4	-4.5	0.0321	0.863 - 0.943	0.830 - 1.141	1.000	876	781
5	25.5	0.0322	0.829 - 1.015	0.792 - 1.134	0.896	4921	4182
6	33.0	0.0347	0.881 - 0.984	0.911 - 1.141	0.830	6635	5131

su = K * Sqrt[sigma^2(I) + (g<I>)^2] where sigma(I) is estimated by SAINT

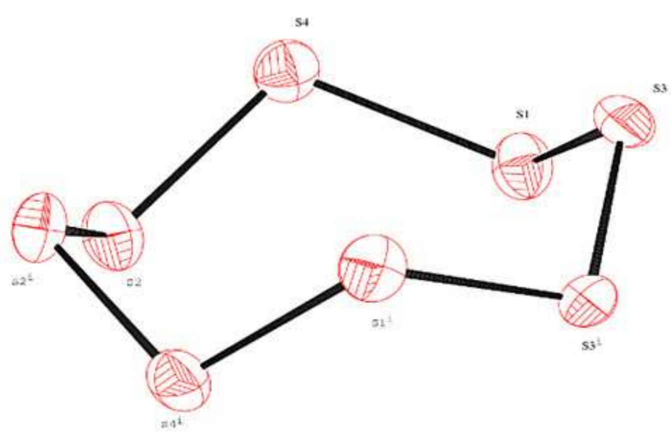

Figure 1

Ortep diagram of sulphur

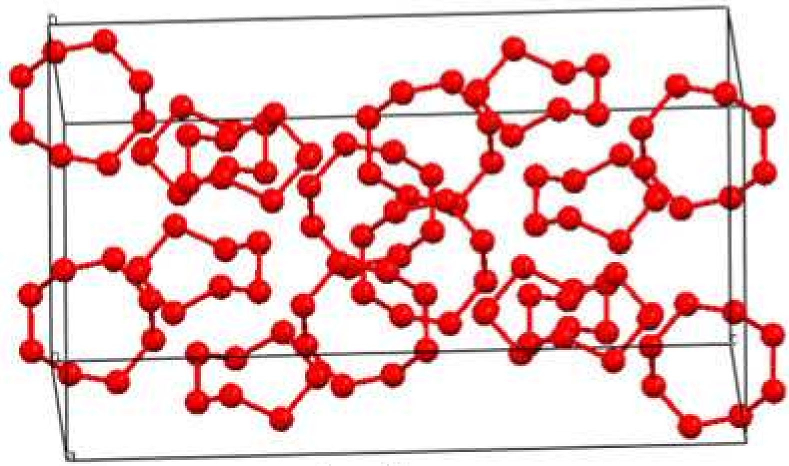

Figure 2

RESULT AND DISCUSSION

The Ortep diagram sulphur molecular structure and Packing diagram respectively shown in the figure .1 and .2.

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