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AS AD No. 400545

400545

# TRANSLATION

METHOD OF OBTAINING A HEAT-RESISTANT PARAMAGNETIC  
POLYMER

By

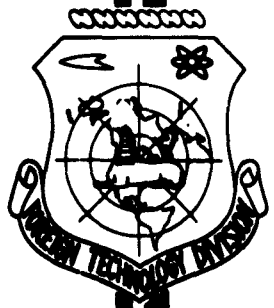
V. P. Parini and A. A. Berlin

## FOREIGN TECHNOLOGY DIVISION

AIR FORCE SYSTEMS COMMAND

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OHIO



## UNEDITED ROUGH DRAFT TRANSLATION

METHOD OF OBTAINING A HEAT-RESISTANT PARAMAGNETIC POLYMER

BY: V. P. Parini and A. A. Berlin

English Pages: 2

SOURCE: Soviet Patent Nr. 148517 (737748/23-4)  
7 July 1961, pp 1

S/19-62-0-13

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METHOD OF OBTAINING A HEAT-RESISTANT PARAMAGNETIC  
POLYMER

V. P. Parini and A. A. Berlin

The familiar method for obtaining a heat-resistant paramagnetic polymer is the reaction of diamine with -p-benzoquinone or its halogen substitute which contains labile hydrogen or halogen atoms adjacent to the carboxylic oxygen.

The proposed method, compared to the familiar method, broadens the source of raw materials for obtaining a heat-resistant paramagnetic polymer. The distinguishing feature of this method is that aromatic diamine is subjected to reaction with quinone, free of labile hydrogen atoms adjacent to the keto group. The polymers thus obtained have increased heat resistance; their specific electrical conductance at 25° is  $10^{-9}$  to  $10^{-7}$   $\text{ohm}^{-1} \text{cm}^{-1}$ , with conductance energy of 0.25 to 0.3 ev.

Example 1. A mixture of 2.7 g (0.05 meta position) of phenylenediamine and 5.2 g (0.05 meta position) of anthraquinone is heated at 300° for 3 hours in a sealed ampoule in an inert atmosphere. The solid product of the reaction is crushed, washed by boiling alcohol,

dried, freed from the low-molecular-weight impurities, and kept at a temperature of 200° and a pressure of 10<sup>-3</sup> mm for 2 hours. The obtained product is black powder which is insoluble in alcohol, acetone, dioxane, and xylene, and which is partly soluble in pyridine, dimethylformamide, and 98% sulfuric acid. The product yield is 5.9 g. At elevated temperatures the obtained paramagnetic polymer undergoes a weight loss: at 400° - 2%, at 500° - 4%, at 600° - 7.5%.

Example 2. A mixture of 2.3 g (0.025 meta position) of benzidine and 2.6 g (0.025 meta position) of anthraquinone is subjected to a reaction as in Example 1. We obtain 3.3 g of a black powder which is insoluble in alcohol, partly soluble in acetone and dioxane, almost completely soluble in pyridine, dimethylformamide, and sulfuric acid, and soluble in 98% sulfuric acid (the solutions have a green color).

Rigid films can be obtained on evaporation of the organic solvents from the solutions. The obtained paramagnetic polymer undergoes the following weight losses with elevated temperatures: at 300° - 2%, at 400° - 5%, and 500° - 8%.

#### Object of the Invention

The method of obtaining a heat-resistant paramagnetic polymer by the reaction of diamine with quinone has the distinguishing feature that in order to expand the raw materials, aromatic diamine is subjected to a reaction with quinone, free of labile hydrogen atoms adjacent to the keto group.

# ORGANIC CHEMISTRY

## ASTIA

DEPUTY FOR SCIENCE & TECHNOLOGY

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74 75 76 77 78 79 80

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DATE 4/22

2ND ANALYST Ret

DATE 4/23

### ALKYL

- |         |       |             |
|---------|-------|-------------|
| 210.1   | 01 0  | ALKANES     |
| 3015.25 | 1     | IC          |
| 1663.25 | 2     | 2C          |
| 3885.25 | 3     | 3C          |
| 0745.25 | 4     | 4C          |
| 3561.25 | 5     | 5C          |
| 2288.25 | 6     | 6C          |
| 2285.25 | 7     | 7C          |
| 3392.25 | 8     | 8C          |
| 3311.25 | 9     | 9C          |
| 1245.5  | 11    | 10C         |
| 0210.11 | 01 12 | 10+C        |
| 0210.14 | 02 0  | TERMINAL    |
| 0210.12 | 1     | NONTERMINAL |
| 0210.13 | 2     | POLY USAGE  |

### ALKENES

- |         |       |             |
|---------|-------|-------------|
| 0210.15 | 3     | ALKENES     |
| 3015.5  | 4     | =CH2        |
| 1663.75 | 5     | C=C         |
| 3885.75 | 6     | 3C          |
| 0745.75 | 7     | 4C          |
| 3561.75 | 8     | 5C          |
| 2288.75 | 9     | 6C          |
| 2285.75 | 11    | 7C          |
| 3392.75 | 02 12 | 8C          |
| 3311.75 | 03 0  | 9C          |
| 1247.5  | 1     | 10C         |
| 0210.16 | 2     | 10+C        |
| 0210.20 | 3     | TERMINAL    |
| 0210.17 | 4     | NONTERMINAL |
| 0210.18 | 5     | POLY =      |
| 0210.19 | 6     | POLY USAGE  |

### ALKYNYL

- |         |       |             |
|---------|-------|-------------|
| 0211.2  | 7     | ALKYNES     |
| 3015.75 | 8     | =C          |
| 0022.5  | 9     | C#C         |
| 3906.5  | 11    | 3C          |
| 0747.5  | 03 12 | 4C          |
| 3565.5  | 04 0  | 5C          |
| 0211.3  | 1     | 6+C         |
| 0211.7  | 2     | TERMINAL    |
| 0211.4  | 3     | NONTERMINAL |
| 0211.5  | 4     | POLY =      |
| 0211.6  | 5     | POLY USAGE  |

### ARYL

- |         |       |            |
|---------|-------|------------|
| 0570.10 | 6     | BENZENE    |
| 0570.15 | 7     | MONOSUB    |
| 0570.11 | 8     | DISUB      |
| 0570.21 | 9     | TRISUB     |
| 0570.16 | 11    | ORTHO      |
| 0570.14 | 04 12 | META       |
| 0570.17 | 05 0  | PARA       |
| 0570.20 | 1     | SYM-TRISUB |
| 0570.19 | 2     | POLYSUB    |
| 0570.13 | 3     | IND        |
| 0570.12 | 4     | FUSED      |
| 0570.18 | 5     | POLY USAGE |

### CYCLOALKANES

- |         |       |              |
|---------|-------|--------------|
| 1225.10 | 6     | CYCLOALKANES |
| 1225.11 | 7     | 3,4M         |
| 1225.12 | 8     | 5M           |
| 1225.13 | 9     | 6M           |
| 1225.14 | 11    | 7+M          |
| 1225.19 | 05 12 | SAT          |
| 1225.21 | 06 0  | UNSAT        |
| 1225.15 | 1     | BICYCLO      |
| 1225.17 | 2     | IND          |
| 1225.16 | 3     | FUSED        |
| 1225.20 | 4     | SPIRO        |
| 1225.18 | 5     | POLY USAGE   |

### HALOGENS

- |        |       |            |
|--------|-------|------------|
| 2214   | 6     | HALOGENS   |
| 1883.2 | 7     | F          |
| 0921.5 | 8     | Cl         |
| 0724.5 | 9     | Br         |
| 2586.5 | 11    | I          |
| 0421   | 06 12 | At         |
| 2214.5 | 07 0  | POLY USAGE |

### CARBONYL

- |         |       |  |
|---------|-------|--|
| 0803.7  | 1     | CARBONYL   |
| 0803.2  | 2     | C=O  |
| 1915.5  | 3     | HC=O   |
| 5091.6  | 4     | C=S  |
| 5091.30 | 5     | HC=S   |
| 3468.25 | 6     | O=(RING)   |
| 5090.11 | 7     | S=(RING)   |
| 2982.5  | 8     | MET. CARBONYLS   |
| 3461.5  | 9     | $\begin{matrix} \text{O} \\   \\ \text{C} \\   \\ \text{O} \end{matrix}$ |
| 0803.5  | 11    | POLY USAGE   |
| 0803.4  | 07 12 | MISC.  |

### COOR

- |         |       |  |
|---------|-------|--|
| 0804.3  | 08 0  | COOR   |
| 0804.1  | 1     | -COO-ESTER   |
| 0804.2  | 2     | COOH   |
| 0804.7  | 3     | CARBOXY HALIDES  |
| 0804.6  | 4     | F-C=O  |
| 0804.5  | 5     | Cl-C=O   |
| 0804.4  | 6     | Br-C=O   |
| 0804.8  | 7     | I-C=O  |
| 0804.9  | 8     | OCOO   |
| 0182.5  | 9     | $\begin{matrix} \text{O} \\   \\ \text{C} \\   \\ \text{O} \end{matrix}$ |
| 0805.25 | 11    | METAL SALT   |
| 0805.75 | 08 12 | POLY USAGE   |
| 0805.5  | 09 0  | MISC.  |

### S-COOR

- |         |       |                   |
|---------|-------|-------------------|
| 5090.15 | 1     | S-COOR            |
| 5090.12 | 2     | THIO ACIDS (CXXH) |
| 5091.5  | 3     | S=C-O             |
| 5091.4  | 4     | O=C-S             |
| 5090.22 | 5     | -S-COOH           |
| 5090.20 | 6     | S=C-HALOGEN       |
| 5090.17 | 7     | S=C-Br            |
| 5090.15 | 8     | S=C-Cl            |
| 5090.19 | 9     | S=C-F             |
| 5090.21 | 11    | S=C-I             |
| 5090.14 | 09 12 | POLY USAGE        |
| 5090.13 | 10 0  | MISC.             |

### S-HETERO

- |         |       |             |
|---------|-------|-------------|
| 4863.10 | 1     | S-HETERO    |
| 4863.14 | 2     | 3, 4M       |
| 4863.15 | 3     | 5M          |
| 4863.16 | 4     | 6M          |
| 4863.17 | 5     | 7+M         |
| 4863.21 | 6     | O-CONT.     |
| 4863.20 | 7     | N-CONT.     |
| 4863.22 | 8     | OTHER-CONT. |
| 4863.11 | 9     | IS          |
| 4863.12 | 11    | 2S          |
| 4863.12 | 10 12 | 3+S         |
| 4863.19 | 11 0  | IND         |
| 4863.18 | 1     | FUSED       |
| 4863.24 | 2     | SPIRO       |
| 4863.23 | 3     | POLY USAGE  |

### N-HETERO

- |         |       |             |
|---------|-------|-------------|
| 3298.10 | 4     | N-HETERO    |
| 3298.14 | 5     | 3, 4M       |
| 3298.15 | 6     | 5M          |
| 3298.16 | 7     | 6M          |
| 3298.17 | 8     | 7+M         |
| 3298.20 | 9     | O-CONT.     |
| 3298.23 | 11    | S-CONT.     |
| 3298.21 | 11 12 | OTHER-CONT. |
| 3298.11 | 12 0  | IN          |
| 3298.12 | 1     | 2N          |
| 3298.13 | 2     | 3+N         |
| 3298.24 | 3     | SALT        |
| 3298.19 | 4     | IND         |
| 3298.18 | 5     | FUSED       |
| 3298.25 | 6     | SPIRO       |
| 3298.22 | 7     | POLY USAGE  |

### O-HETERO

- |         |       |             |
|---------|-------|-------------|
| 3475.10 | 8     | O-HETERO    |
| 3475.13 | 9     | 3, 4M       |
| 3475.14 | 11    | 5M          |
| 3475.15 | 12 12 | 6M          |
| 3475.16 | 13 0  | 7+M         |
| 3475.19 | 1     | N-CONT.     |
| 3475.22 | 2     | S-CONT.     |
| 3475.20 | 3     | OTHER-CONT. |
| 3475.11 | 4     | I-O         |
| 3475.12 | 5     | 2+O         |
| 3475.18 | 6     | IND         |
| 3475.17 | 7     | FUSED       |
| 3475.23 | 8     | SPIRO       |
| 3475.21 | 9     | POLY USAGE  |

### N, C, S

- |         |       |             |
|---------|-------|-------------|
| 3297.5  | 11    | N,C,S       |
| 5090.16 | 13 12 | =N-C=S      |
| 1398.75 | 14 0  | -N-C(-S)-S  |
| 5091.7  | 1     | =N-C(=S)-NE |
| 5091.20 | 2     | -S-CN       |
| 2618.5  | 3     | -N=C=S      |
| 3297.7  | 4     | POLY USAGE  |
| 3297.6  | 5     | MISC.       |

### N, C, O

- |         |       |             |
|---------|-------|-------------|
| 3297.2  | 6     | N,C,O       |
| 4462.5  | 7     | NC(=O)-N-N  |
| 0785.25 | 8     | -N-C(-O)-O- |
| 5361.5  | 9     | =N-C(=O)-N- |
| 0785.75 | 11    | -C(=O)-N-   |
| 2613.25 | 14 12 | -N=C=O      |
| 1222.5  | 15 0  | -O-CN       |
| 3297.4  | 1     | POLY USAGE  |
| 3297.3  | 2     | MISC.       |

### C, N

- |         |    |             |
|---------|----|-------------|
| 0797.25 | 3  | C,N         |
| 1223.5  | 4  | CN          |
| 2613.75 | 5  | -N=C        |
| 0239.2  | 6  | -N-C=N      |
| 2150.5  | 7  | -N-C(=N)-N- |
| 0787.5  | 8  | -N=C=N-     |
| 0797.75 | 9  | POLY USAGE  |
| 0797.5  | 11 | MISC.       |

### OH, SH

- |         |       |            |
|---------|-------|------------|
| 2391.6  | 15 12 | OH, SH     |
| 2391.4  | 16 0  | OH         |
| 2968.25 | 1     | SH         |
| 2391.8  | 2     | POLY USAGE |

### N, O, (S)

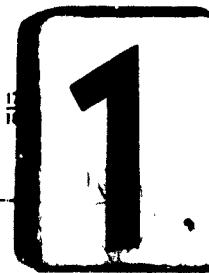
- |         |       |            |
|---------|-------|------------|
| 3298.27 | 3     | N,O(S)     |
| 2391.2  | 4     | =N-OH      |
| 2968.75 | 5     | =N-SH      |
| 3295.5  | 6     | NO2        |
| 3299.75 | 7     | -N=O       |
| 3299.25 | 8     | -N=N=C     |
| 3289.5  | 9     | N-NO2      |
| 3298.29 | 11    | POLY USAGE |
| 3298.27 | 16 12 | MISC.      |

### S, O, (N)

- |         |      |            |
|---------|------|------------|
| 4863.25 | 17 0 | S, O(N)    |
| 4860.75 | 1    | O=S=O      |
| 4860.25 | 2    | SO3H       |
| 4859.5  | 3    | S=O        |
| 4860.5  | 4    | SO2-N      |
| 4863.27 | 5    | POLY USAGE |
| 4863.26 | 6    | MISC.      |

### O, S

- |         |   |     |
|---------|---|-----|
| 3468.75 | 1 | O,S |
| 3587.5  | 2 | O,S |
| 5090.10 | 3 | O,S |
| 1398.25 | 4 | O,S |
| 5257.5  | 5 | O,S |
| 3475.28 | 6 | O,S |



# IC CHEMISTRY

## ASTIA

### SCIENCE & TECHNOLOGY

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S - HETERO	
4863.10	1 S-HETERO
4863.14	2 3, 4M
4863.15	3 5M
4863.16	4 6M
4863.17	5 7+M
4863.21	6 O-CONT.
4863.20	7 N-CONT.
4863.22	8 OTHER-CONT.
4863.11	9 IS
4863.12	11 2S
4863.12	10 12 3+S
4863.19	11 0 IND
4863.18	1 FUSED
4863.24	2 SPIRO
4863.23	3 POLY USAGE

N - HETERO	
3298.10	4 N-HETERO
3298.14	5 3, 4M
3298.15	6 5M
3298.16	7 6M
3298.17	8 7+M
3298.20	9 O-CONT.
3298.23	11 S-CONT.
3298.21	11 12 OTHER-CONT.
3298.11	12 0 IN
3298.12	1 2N
3298.13	2 3+N
3298.24	3 SALT
3298.19	4 IND
3298.18	5 FUSED
3298.25	6 SPIRO
3298.22	7 POLY USAGE

O-HETERO	
3475.10	8 O-HETERO
3475.13	9 3, 4M
3475.14	11 5M
3475.15	12 12 6M
3475.16	13 0 7+M
3475.19	1 N-CONT.
3475.22	2 S-CONT.
3475.20	3 OTHER-CONT.
3475.11	4 I-O
3475.12	5 2+O
3475.18	6 IND
3475.17	7 FUSED
3475.23	8 SPIRO
3475.21	9 POLY USAGE

3297.5  
5090.16  
1398.75  
5001.7  
5001.20  
2618.5  
3297.7  
3297.6

3297.2  
4462.5  
0785.25  
5361.5  
0785.75  
2613.25  
1222.5  
3297.4  
3297.3

0797.25  
1223.5  
2613.75  
0239.2  
2150.5  
0787.5  
0797.75  
0797.5

2391.6  
2391.4  
2968.25  
2391.8

3298.27  
2391.2  
2968.75  
3295.5  
3299.75  
3299.25  
3289.5  
3298.29  
3298.27

4863.25  
4860.75  
4860.25  
4859.5  
4860.5  
4863.27  
4863.26

4863.25  
3587.5  
5090.10  
1398.25  
5257.5  
3475.28

#### N, C, S

11 N,C,S  
13 12 =N-C-S  
14 0 =N-C(=S)-S  
1 =N-C(=S)-NE  
2 -S-CN  
3 -N=C=S  
4 POLY USAGE  
5 MISC.

#### N, C, O

6 N,C,C  
7 NC(=O)-N-N  
8 -N-C(=O)-O-  
9 =N-C(=O)-N-  
11 -C(=O)-N-  
14 12 -N=C=O  
15 0 -O-CN  
1 POLY USAGE  
2 MISC.

#### C, N

3 C,N  
4 CN  
5 =N=C  
6 -N-C=N  
7 -N-C(=N)-N-  
8 -N=C=N-  
9 POLY USAGE  
11 MISC.

#### OH, SH

15 12 OH, SH  
16 0 OH  
1 SH  
2 POLY USAGE

#### N, O, (S)

3 N,O (S)  
4 =N-OH  
5 =N-SH  
6 NO2  
7 -N=O  
8 -N=N=C  
9 N-NO2  
11 POLY USAGE  
16 12 MISC.

#### S, O, (N)

17 0 S, O (N)  
1 O=S=O  
2 SO3H  
3 S=O  
4 SO2-N  
5 POLY USAGE  
6 MISC.

#### O, S

7 O,S  
8 -O-  
9 -O-O-  
11 -S-  
17 12 -S-S-  
18 0 -S-S-S-  
1 POLY USAGE  
2 MISC.

#### AMINES

0239.5  
3852.5  
4442.5  
5036.5  
3984.5  
2442.5  
0503.5  
1329.5  
2359.5  
5251.5  
0501.5

3 AMINES  
4 NH2 (PRI)  
5 -NH- (SEC)  
6 -N= (TER)  
7 -N= (QUAT)  
8 =N  
9 -N=N-  
11 N=N (N=N)  
12 -N-N-  
19 0 N-N=N-  
1 N=N  
2 FLUROAMINES  
3 -NF2  
4 -NF  
5 F2N-NF-  
6 SALT (NON-QUAT)  
7 POLY USAGE  
8 MISC.

#### PHOSPHORUS

3634.2  
3634.16  
3634.18  
3634.17  
3634.19  
3634.15  
3634.14  
3634.11  
3634.10  
3634.13  
3634.12  
3634.23  
3634.24  
1224.75  
3632.25  
3632.75  
3617.5  
3634.21  
3634.25  
3634.22

9 PHOSPHORUS RAD.  
11 P=O,S,O  
19 12 P=S,2O  
20 0 P=O, S, 2O  
1 S=PO3  
2 S=P-F  
3 S=P-F  
4 O=P(N) (O)-F  
5 O=P, (F), 2N  
6 O=P(F) O2  
7 O=P-F  
8 P,S-(1 TO 3S)  
9 P,S-(4S)  
11 CYCLIC P  
20 12 P(+3)  
21 0 P(+5)  
1 PO4  
2 P-MISC.  
3 P,S-MISC.  
4 POLY USAGE

#### BORANES

0687  
4530

#### SILANES

#### MISCELLANEOUS

22 23  
0 0  
1 1  
2 2  
3 3  
4 4  
5 5  
6 6  
7 7  
8 8  
9 9  
11 11  
12 12

#### METALS AND METALLOIDS

2140  
0205  
0877  
1925  
2787  
3805  
4592  
4365  
1134  
2102  
4542

24 0 GROUP I  
1 ALKALI  
2 Cs  
3 Fr  
4 Li  
5 K  
6 Na  
7 Rb  
8 Cu  
9 Au  
11 Ag

2141  
0208  
0536  
0573  
0760  
2845  
4110  
4821  
0755  
0970  
5585

24 12 GROUP II  
25 0 ALKALINE  
1 Ba  
2 Be  
3 Ca  
4 Mg  
5 Ra  
6 Sn  
7 Co  
8 Hg  
9 Zn

2142  
0043  
0232  
1996  
2467  
2707  
4410  
5055  
5583

11 GROUP III  
25 12 Ac  
26 0 Al  
1 Ga  
2 In  
3 La  
4 Sc  
5 Tl  
6 Y

2143  
2072  
2201  
2719  
5128  
5139  
5590

7 GROUP IV  
8 Ge  
9 Hf  
11 Pb  
26 12 Sn  
27 0 Ti  
1 Zr

2144  
0330  
0610  
3287  
4956  
5381

2 GROUP V  
3 Sb  
4 Bi  
5 Nb  
6 P  
7 Ta  
8 V

2145  
0883  
3781  
4457  
0935  
3122  
5277

9 GROUP VI  
11 CHALCOGENS  
27 12 Po  
28 0 Sr  
1 Cr  
2 Mo  
3 W

2146  
5223  
0992  
2604  
2607  
3276  
3456  
3492  
3744  
4277  
4373

4 GROUP VII  
5 TRANS. ELEM.  
6 Co  
7 In  
8 Fe  
9 Ni  
11 Os  
28 12 Pb  
29 0 Pt  
1 Rh  
2 Ru



# FRAGMENT RELATIONSHIPS

[ALKYL]	[ALKENYL]	[ALKYNYL]	[ARYL]	[CYCLOALKYL]	[H]
30 0 ARYL 1 CYCLOALKYL 2 HALOGENS 3 CARBONYL 4 COOR 5 S-COOR 6 S-HETERO 7 N-HETERO 8 O-HETERO 9 N,C,S 11 N,C,O 30 12 C,N 31 0 N,O(S) 1 OH, SH 2 S,O(N) 3 O,S 4 AMINES 5 PHOSPHORUS 6 METALS 7 BORANES 8 SILANES 9 MISC.	11 ARYL 31 12 CYCLOALKYL 32 0 HALOGENS 1 CARBONYL 2 COOR 3 S-COOR 4 S-HETERO 5 N-HETERO 6 O-HETERO 7 N,C,S 8 N,C,O 9 C,N 11 N,O(S) 32 12 OH, SH 33 0 S,O(N) 1 O,S 2 AMINES 3 PHOSPHORUS 4 METALS 5 BORANES 6 SILANES 7 MISC.	8 ARYL 9 CYCLOALKYL 11 HALOGENS 33 12 CARBONYL 34 0 COOR 1 S-COOR 2 S-HETERO 3 N-HETERO 4 O-HETERO 5 N,C,S 6 N,C,O 7 C,N 8 N,O(S) 9 OH, SH 11 S,O(N) 34 12 O,S 35 0 AMINES 1 PHOSPHORUS 2 METALS 3 BORANES 4 SILANES 5 MISC.	6 ARYL 7 CYCLOALKYL 8 HALOGENS 9 CARBONYL 11 COOR 35 12 S-COOR 36 0 S-HETERO 1 N-HETERO 2 O-HETERO 3 N,C,S 4 N,C,O 5 C,N 6 N,O(S) 7 OH, SH 8 S,O(N) 9 O,S 11 AMINES 36 12 PHOSPHORUS 37 0 METALS 1 BORANES 2 SILANES 3 MISC.	4 CYCLOALKYL 5 HALOGENS 6 CARBONYL 7 COOR 8 S-COOR 9 S-HETERO 11 N-HETERO 37 12 O-HETERO 38 0 N,C,S 1 N,C,O 2 C,N 3 N,O(S) 4 OH, SH 5 S,O(N) 6 O,S 7 AMINES 8 PHOSPHORUS 9 METALS 11 BORANES 38 12 SILANES 39 0 MISC.	1 2 3 4 5 6 7 8 9 11 12 39 40 0 1 2 3 4 5 6 7 8 9

[S-HETERO]	[N-HETERO]	[O-HETERO]	[N,C,S]	[N,C,O]	[H]
44 0 S-HETERO 1 N-HETERO 2 O-HETERO 3 N,C,S 4 N,C,O 5 C,N 6 N,O(S) 7 OH, SH 8 S,O(N) 9 O,S 11 AMINES 44 12 PHOSPHORUS 45 0 METALS 1 BORANES 2 SILANES 3 MISC.	4 N-HETERO 5 O-HETERO 6 N,C,S 7 N,C,O 8 C,N 9 N,O(S) 11 OH, SH 45 12 S,O(N) 46 0 O,S 1 AMINES 2 PHOSPHORUS 3 METALS 4 BORANES 5 SILANES 6 MISC.	7 O-HETERO 8 N,C,S 9 N,C,O 11 C,N 46 12 N,O(S) 47 0 OH, SH 1 S,O(N) 2 O,S 3 AMINES 4 PHOSPHORUS 5 METALS 6 BORANES 7 SILANES 8 MISC.	9 N,C,S 11 N,C,O 47 12 C,N 48 0 N,O(S) 1 OH, SH 2 S,O(N) 3 O,S 4 AMINES 5 PHOSPHORUS 6 METALS 7 BORANES 8 SILANES 9 MISC.	11 N,C,O 48 12 C,N 49 0 N,O(S) 1 OH, SH 2 S,O(N) 3 O,S 4 AMINES 5 PHOSPHORUS 6 METALS 7 BORANES 8 SILANES 9 MISC.	11 49 12 50 0 1 2 3 4 5 6 7 8 9

<p style="font-size: 2em; font-weight: bold; margin: 0;">AD</p> <table style="margin: 5px auto; border-collapse: collapse;"> <tr> <td style="border: 1px solid black; width: 20px; height: 20px; text-align: center;">9</td> <td style="border: 1px solid black; width: 20px; height: 20px; text-align: center;">0</td> <td style="border: 1px solid black; width: 20px; height: 20px; text-align: center;">0</td> <td style="border: 1px solid black; width: 20px; height: 20px; text-align: center;">5</td> <td style="border: 1px solid black; width: 20px; height: 20px; text-align: center;">4</td> <td style="border: 1px solid black; width: 20px; height: 20px; text-align: center;">5</td> </tr> <tr> <td style="text-align: center;">74</td> <td style="text-align: center;">75</td> <td style="text-align: center;">76</td> <td style="text-align: center;">77</td> <td style="text-align: center;">78</td> <td style="text-align: center;">79</td> </tr> </table>	9	0	0	5	4	5	74	75	76	77	78	79	<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="width: 25%;">[O,S]</th> <th style="width: 25%;">[AMINES]</th> <th style="width: 25%;">[PHOSPHORUS]</th> <th style="width: 25%;">[H]</th> </tr> </thead> <tbody> <tr> <td>                             52                              O,S                              6 AMINES                              PHOSPHORUS                              7 METALS                              8 BORANES                              9 SILANES                              11 MISC.                         </td> <td>                             AMINES                              52 12 PHOSPHORUS                              53 0 METALS                              1 BORANES                              2 SILANES                              3 MISC.                         </td> <td>                             PHOSPHORUS                              4 METALS                              5 BORANES                              6 SILANES                              7 MISC.                         </td> <td>                             53 12 5 11 53 12                         </td> </tr> </tbody> </table>	[O,S]	[AMINES]	[PHOSPHORUS]	[H]	52 O,S 6 AMINES PHOSPHORUS 7 METALS 8 BORANES 9 SILANES 11 MISC.	AMINES 52 12 PHOSPHORUS 53 0 METALS 1 BORANES 2 SILANES 3 MISC.	PHOSPHORUS 4 METALS 5 BORANES 6 SILANES 7 MISC.	53 12 5 11 53 12
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[O,S]	[AMINES]	[PHOSPHORUS]	[H]																		
52 O,S 6 AMINES PHOSPHORUS 7 METALS 8 BORANES 9 SILANES 11 MISC.	AMINES 52 12 PHOSPHORUS 53 0 METALS 1 BORANES 2 SILANES 3 MISC.	PHOSPHORUS 4 METALS 5 BORANES 6 SILANES 7 MISC.	53 12 5 11 53 12																		

RING SYSTEM (GENERAL)	RING INDEX NO.	RING INDEX NAME																																														
<table style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 50%; vertical-align: top;">                             4292. 2                              4292. 4                              4292. 5                              4292. 7                              4292. 9                              3298. 29                              3298. 30                              3298. 31                              4863. 28                              4863. 29                              3475. 24                              3475. 25                              3089. 25                              3089. 75                         </td> <td style="width: 50%; vertical-align: top;">                             6 RINGS-2                              7 RINGS-3                              8 RINGS-4                              9 RINGS-5                              11 RINGS-6+                              54 12 N-RINGS-1                              55 0 N-RINGS-2                              1 N-RINGS-3+                              2 S-RINGS-1                              3 S-RINGS-2+                              4 O-RINGS-1                              5 O-RINGS-2+                              6 MISC. -HETERO RINGS-1                              7 MISC. -HETERO RINGS-2                         </td> </tr> </table>	4292. 2 4292. 4 4292. 5 4292. 7 4292. 9 3298. 29 3298. 30 3298. 31 4863. 28 4863. 29 3475. 24 3475. 25 3089. 25 3089. 75	6 RINGS-2 7 RINGS-3 8 RINGS-4 9 RINGS-5 11 RINGS-6+ 54 12 N-RINGS-1 55 0 N-RINGS-2 1 N-RINGS-3+ 2 S-RINGS-1 3 S-RINGS-2+ 4 O-RINGS-1 5 O-RINGS-2+ 6 MISC. -HETERO RINGS-1 7 MISC. -HETERO RINGS-2	<table style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 25%;">56</td> <td style="width: 25%;">57</td> <td style="width: 25%;">58</td> <td style="width: 25%;">59</td> </tr> <tr> <td style="text-align: center;">0</td> <td style="text-align: center;">0</td> <td style="text-align: center;">0</td> <td style="text-align: center;">0</td> </tr> <tr> <td style="text-align: center;">1</td> <td style="text-align: center;">1</td> <td style="text-align: center;">1</td> <td style="text-align: center;">1</td> </tr> <tr> <td style="text-align: center;">2</td> <td style="text-align: center;">2</td> <td style="text-align: center;">2</td> <td style="text-align: center;">2</td> </tr> <tr> <td style="text-align: center;">3</td> <td style="text-align: center;">3</td> <td style="text-align: center;">3</td> <td style="text-align: center;">3</td> </tr> <tr> <td style="text-align: center;">4</td> <td style="text-align: center;">4</td> <td style="text-align: center;">4</td> <td style="text-align: center;">4</td> </tr> <tr> <td style="text-align: center;">5</td> <td style="text-align: center;">5</td> <td style="text-align: center;">5</td> <td style="text-align: center;">5</td> </tr> <tr> <td style="text-align: center;">6</td> <td style="text-align: center;">6</td> <td style="text-align: center;">6</td> <td style="text-align: center;">6</td> </tr> <tr> <td style="text-align: center;">7</td> <td style="text-align: center;">7</td> <td style="text-align: center;">7</td> <td style="text-align: center;">7</td> </tr> <tr> <td style="text-align: center;">8</td> <td style="text-align: center;">8</td> <td style="text-align: center;">8</td> <td style="text-align: center;">8</td> </tr> <tr> <td style="text-align: center;">9</td> <td style="text-align: center;">9</td> <td style="text-align: center;">9</td> <td style="text-align: center;">9</td> </tr> </table>	56	57	58	59	0	0	0	0	1	1	1	1	2	2	2	2	3	3	3	3	4	4	4	4	5	5	5	5	6	6	6	6	7	7	7	7	8	8	8	8	9	9	9	9	<div style="border: 2px solid black; padding: 10px; font-size: 4em; font-weight: bold; width: 60px; margin: 0 auto;">1</div>
4292. 2 4292. 4 4292. 5 4292. 7 4292. 9 3298. 29 3298. 30 3298. 31 4863. 28 4863. 29 3475. 24 3475. 25 3089. 25 3089. 75	6 RINGS-2 7 RINGS-3 8 RINGS-4 9 RINGS-5 11 RINGS-6+ 54 12 N-RINGS-1 55 0 N-RINGS-2 1 N-RINGS-3+ 2 S-RINGS-1 3 S-RINGS-2+ 4 O-RINGS-1 5 O-RINGS-2+ 6 MISC. -HETERO RINGS-1 7 MISC. -HETERO RINGS-2																																															
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## FRAGMENT RELATIONSHIPS

	<b>[ARYL]</b>	<b>[CYCLOALKYL]</b>	<b>[HALOGENS]</b>	<b>[CARBONYL]</b>	<b>[S-COOR]</b>	<b>[COOR]</b>
.KYL IS L	6 ARYL 7 CYCLOALKYL 8 HALOGENS 9 CARBONYL 11 COOR 35 12 S-COOR 36 0 S-HETERO 1 N-HETERO 2 O-HETERO 3 N,C,S 4 N,C,O 5 C,N 6 N,O(S) 7 OH, SH 8 S,O(N) 9 O,S 11 AMINES 36 12 PHOSPHORUS 37 0 METALS 1 BORANES 2 SILANES 3 MISC.	4 CYCLOALKYL 5 HALOGENS 6 CARBONYL 7 COOR 8 S-COOR 9 S-HETERO 11 N-HETERO 37 12 O-HETERO 38 0 N,C,S 1 N,C,O 2 C,N 3 N,O(S) 4 OH, SH 5 S,O(N) 6 O,S 7 AMINES 8 PHOSPHORUS 9 METALS 11 BORANES 38 12 SILANES 39 0 MISC.	1 HALOGENS 2 CARBONYL 3 COOR 4 S-COOR 5 S-HETERO 6 N-HETERO 7 O-HETERO 8 N,C,S 9 N,C,O 11 C,N 12 N,O(S) 39 OH, SH 40 0 S,O(N) 1 O,S 2 AMINES 3 PHOSPHORUS 4 METALS 5 BORANES 6 SILANES 7 MISC.	8 CARBONYL 9 S-COOR 11 S-HETERO 40 12 N-HETERO 41 0 O-HETERO 1 N,C,S 2 N,C,O 3 C,N N,O(S) OH, SH 4 S,O(N) O,S AMINES 5 PHOSPHORUS 6 METALS 7 BORANES 8 SILANES 9 MISC.	11 COOR 41 12 S-COOR 42 0 S-HETERO 1 N-HETERO 2 O-HETERO 3 N,C,S N,C,O C,N N,O(S) OH, SH S,O(N) 4 O,S 5 AMINES 6 PHOSPHORUS 7 METALS 8 BORANES 9 SILANES 11 MISC.	42 12 S-HETERO 43 0 N-HETERO 1 O-HETERO 2 N,C,S 3 N,C,O 4 C,N N,O(S) OH, SH S,O(N) 5 O,S 6 AMINES 7 PHOSPHORUS 8 METALS 9 BORANES 11 SILANES 43 12 MISC.
TO TO TO						
ORUS						
S						
RO	<b>[N,C,S]</b>	<b>[N,C,O]</b>	<b>[C,N]</b>	<b>[N,O(S)]</b>	<b>[OH, SH]</b>	<b>[S,O(N)]</b>
	9 N,C,S 11 N,C,O 47 12 C,N 48 0 N,O(S) 1 OH, SH 2 S,O(N) 3 O,S 4 AMINES 5 PHOSPHORUS 6 METALS 7 BORANES 8 SILANES 9 MISC.	11 N,C,O 48 12 C,N 49 0 N,O(S) 1 OH, SH 2 S,O(N) 3 O,S 4 AMINES 5 PHOSPHORUS 6 METALS 7 BORANES 8 SILANES 9 MISC.	11 C,N 49 12 N,O(S) 50 0 OH, SH 1 S,O(N) 2 O,S 3 AMINES 4 PHOSPHORUS 5 METALS 6 BORANES 7 SILANES 8 MISC.	N,O(S) OH, SH 9 S,O(N) O,S 11 AMINES 50 12 PHOSPHORUS 51 0 METALS 1 BORANES 2 SILANES 3 MISC.	51 4 OH, SH S,O(N) O,S 5 AMINES 6 PHOSPHORUS 7 METALS 8 BORANES 9 SILANES 11 MISC.	S,O(N) 51 12 O,S 52 0 AMINES 1 PHOSPHORUS 2 METALS 3 BORANES 4 SILANES 5 MISC.
ORUS						
S						
ORUS	<b>[AMINES]</b>	<b>[PHOSPHORUS]</b>	<b>[METALS]</b>	<b>[BORANES]</b>	<b>[SILANES]</b>	<b>[MISC.]</b>
	AMINES 52 12 PHOSPHORUS 53 0 METALS 1 BORANES 2 SILANES 3 MISC.	53 PHOSPHORUS 4 METALS 5 BORANES 6 SILANES 7 MISC.	8 METALS 9 BORANES 11 SILANES 53 12 MISC.	54 0 BORANES 1 SILANES 2 MISC.	54 3 SILANES 4 MISC.	54 5 MISC.
ORUS						
S						

X NO.	RING INDEX NAME	OPEN-ENDED SECTION
59 0 1 2 3 4 5 6 7 8 9		COL & ROW  SECTION  <div style="border: 2px solid black; padding: 10px; font-size: 48px; font-weight: bold; text-align: center; width: 100px; margin: 0 auto;">2</div>

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