**List of reactions**

**Gas-phase reactions**

|  |  |
| --- | --- |
| Reaction1 | Geranylacetone+O3**→**(1/4)((BR2)CI1+(BR2)CI2+(BR1)CI7+(BR1)CI8+(BR1)acetone+(BR1)6-MHO+(BR2)4-MON+(BR2)4-OPA) |
| Reaction2 | 6-MHO+O3**→**(1/2)((BR2)CI1+(BR1)CI7+(BR1)acetone+(BR2)4-OPA) |
| Reaction3 | 4-MON+O3**→**(1/2)((BR1)CI7+(BR2)CI12+(BR2)4-OPA+(BR1)4-OPA) |
| Reaction4 | 4-MOD+O3**→**(1/2)((BR1)CI9+(BR2)CI12+(BR1)4-OPA+(BR2)butanedial) |
| Reaction5 | HK3+O3**→**(1/2)((BR2)CI1+(BR1)CI20+(BR1)acetone+(BR2)HK2) |
| Reaction6 | CI1+H2O**→**acetone |
| Reaction7 | CI1+O3**→**acetone |
| Reaction8 | CI1**→**HK1 |
| Reaction9 | CI2+H2O**→**6-MHO |
| Reaction10 | CI2+O3**→**6-MHO |
| Reaction11 | CI2**→**HK3 |
| Reaction12 | CI7+H2O**→**4-OPA |
| Reaction13 | CI7+O3**→**4-OPA |
| Reaction14 | CI7**→**CA1 |
| Reaction15 | CI8+H2O**→**4-MON |
| Reaction16 | CI8+O3**→**4-MON |
| Reaction17 | CI8**→**Product |
| Reaction18 | CI9+H2O**→**butanedial |
| Reaction19 | CI9+O3**→**butanedial |
| Reaction20 | CI9**→**CA2 |
| Reaction21 | CI12+H2O**→**4-OPA |
| Reaction22 | CI12+O3**→**4-OPA |
| Reaction23 | CI12**→**HK2 |
| Reaction24 | CI20+H2O**→**HK2 |
| Reaction25 | CI20+O3**→**HK2 |
| Reaction26 | CI20**→**Product |

**Condensed-phase reactions**

|  |  |
| --- | --- |
| Reaction1 | Squalene+O3**→**(1/6)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)CI4+(BR1)CI5+(BR1)CI6+(BR2)TOT+(BR2)TOP+(BR2)TTT+(BR1)Geranylacetone+(BR1)6-MHO+(BR1)acetone) |
| Reaction2 | 6-MHO+O3**→**(1/2)((BR2)CI1+(BR1)Product+(BR1)acetone+(BR2)4-OPA) |
| Reaction3 | Geranylacetone+O3**→**(1/4)((BR2)CI1+(BR2)CI2+(BR1)Product+(BR1)Product+(BR1)acetone+(BR1)6-MHO+(BR2)4-MON+(BR2)4-OPA) |
| Reaction4 | TTT+O3**→**(1/6)((BR2)CI1+(BR2)CI2+(BR2)CI3+((BR1)Product+(BR1)Product+(BR1)Product+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)ProductA+(BR2)4-MOD+(BR2)butanedial) |
| Reaction5 | 4-MON+O3**→**(1/2)((BR1)Product+(BR2)CI12+(BR2)4-OPA+(BR1)4-OPA) |
| Reaction6 | 4-MOD+O3**→**(1/2)((BR1)Product+(BR2)CI12+(BR1)4-OPA+(BR2)butanedial) |
| Reaction7 | ProductA+O3**→**(1/4)((BR1)Product+(BR1)Product+(BR2)CI12+(BR2)CI16+(BR1)4-OPA+(BR1)4-MON+(BR2)4-MOD+(BR2)butanedial) |
| Reaction8 | TOP+O3**→**(1/8)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)CI4+(BR2)CI12+(BR1)Product+(BR1)Product+(BR1)Product+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR1)4-OPA+(BR2)4-MOD+(BR2)ProductB+(BR2)ProductC) |
| Reaction9 | ProductB+O3**→**(1/4)((BR2)CI12+(BR2)CI12+(BR1)Product+(BR1)Product+((BR1)4-OPA+(BR1)4-OPA+(BR2)4-MOD+(BR2)4-MOD) |
| Reaction10 | ProductC+O3**→**(1/6)((BR2)CI12+(BR2)CI12+(BR1)Product+(BR1)Product+(BR2)CI16+(BR1)Product+(BR1)4-OPA+(BR1)4-OPA+(BR1)4-MON+(BR2)ProductA+(BR2)4-MOD+(BR2)ProductB) |
| Reaction11 | TOT+O3**→**(1/10)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)CI4+(BR1)CI5+(BR2)CI12+(BR2)CI16+(BR1)Product+(BR1)Product+(BR1)Product+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)TTT+(BR2)TOP+(BR2)ProductD+(BR2)ProductC+(BR2)ProductA+(BR1)4-MON+(BR1)4-OPA) |
| Reaction12 | ProductD+O3**→**(1/4)((BR2)CI12+(BR2)CI16+(BR1)Product+(BR1)Product+(BR1)4-OPA+(BR1)4-MON+(BR2)ProductA+(BR2)ProductC) |
| Reaction13 | HK3+O3**→**(1/2)((BR2)CI1+(BR1)Product+(BR1)acetone+(BR2)HK2) |
| Reaction14 | HK5+O3**→**(1/4)((BR2)CI1+(BR2)CI2+(BR1)Product+(BR1)Product+(BR1)acetone+(BR1)6-MHO+(BR2)HK2+(BR2)HK4) |
| Reaction15 | CA9+O3**→**(1/6)((BR2)CI1+(BR2)CI2+(BR2)CI3+(BR1)Product+(BR1)Product+(BR1)Product+(BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)CA2+(BR2)CA5+(BR2)CA8) |
| Reaction16 | CI1+H2O**→**acetone |
| Reaction17 | CI1+O3**→**acetone |
| Reaction18 | CI1**→**HK1 |
| Reaction19 | CI1+allcarbonyl**→**Product |
| Reaction20 | CI12+H2O**→**4-OPA |
| Reaction21 | CI12+O3**→**4-OPA |
| Reaction22 | CI12**→**HK2 |
| Reaction23 | CI12+allcarbonyl**→**SOorHP4 |
| Reaction24 | CI2+H2O**→**6-MHO |
| Reaction25 | CI2+O3**→**6-MHO |
| Reaction26 | CI2**→**HK3 |
| Reaction27 | CI2+allcarbonyl**→**SOorHP5 |
| Reaction28 | CI16+H2O**→**4-MON |
| Reaction29 | CI16+O3**→**4-MON |
| Reaction30 | CI16**→**Product |
| Reaction31 | CI16+allcarbonyl**→**SOorHP9 |
| Reaction32 | CI3+H2O**→**Geranylacetone |
| Reaction33 | CI3+O3**→**Geranylacetone |
| Reaction34 | CI3**→**HK5 |
| Reaction35 | CI3+allcarbonyl**→**SOorHP10 |
| Reaction36 | CI4+H2O**→**TTT |
| Reaction37 | CI4+O3**→**TTT |
| Reaction38 | CI4**→**CA9 |
| Reaction39 | CI4+allcarbonyl**→**SOorHP14 |
| Reaction40 | CI5+H2O**→**TOP |
| Reaction41 | CI5+O3**→**TOP |
| Reaction42 | CI5**→**Product |
| Reaction43 | CI5+allcarbonyl**→**Product |
| Reaction44 | CI6+H2O**→**TOT |
| Reaction45 | CI6+O3**→**TOT |
| Reaction46 | CI6**→**Product |
| Reaction47 | CI6+allcarbonyl**→**Product |
| Reaction48 | 6-MHO+allCI**→**SOorHP5 |
| Reaction49 | Geranylacetone+allCI**→**SOorHP10 |
| Reaction50 | TTT+allCI**→**SOorHP14 |
| Reaction51 | TOP+allCI**→**Product |
| Reaction52 | TOT+allCI**→**Product |
| Reaction53 | 4-MON+allCI**→**SOorHP6+SOorHP9 |
| Reaction54 | 4-MOD+allCI**→**SOorHP7+SOorHP8 |
| Reaction55 | ProductA+allCI**→**Product+Product |
| Reaction56 | ProductB+allCI**→**Product |
| Reaction57 | ProductC+allCI**→**Product+Product |
| Reaction58 | ProductD+allCI**→**Product |
| Reaction59 | CA1+allCI**→**Product |
| Reaction60 | CA2+allCI**→**Product |
| Reaction61 | Removed |
| Reaction62 | Removed |
| Reaction63 | Removed |
| Reaction64 | HK2+allCI**→**Product+Product |
| Reaction65 | HK3+allCI**→**Product |
| Reaction66 | Removed |
| Reaction67 | HK5+allCI**→**Product |
| Reaction68 | SO or HP5+O3**→**(1/2)((BR1)acetone+(BR2)SO or HP4+(BR1)Product+(BR2)CI1) |
| Reaction69 | SO or HP6+O3**→**(1/2)((BR2)4-OPA+(BR1)Product+(BR1)SO or HP2+(BR2)CISO or CIHP2) |
| Reaction70 | SO or HP7+O3**→**(1/2)((BR2)butanedial+(BR1)Product+(BR1)SOor HP2+(BR2)CISO or CIHP2) |
| Reaction71 | SO or HP8+O3**→**(1/2)((BR1)4-OPA+(BR2)CI12+(BR2)SO or HP3+(BR1)Product) |
| Reaction72 | SO or HP9+O3**→**(1/2)((BR1)4-OPA+(BR2)CI12+(BR2)SO or HP4+(BR1)Product) |
| Reaction73 | SO or HP10+O3**→**(1/4)((BR1)acetone+(BR1)6-MHO+(BR2)CI1+(BR2)CI2+(BR2)SO or HP4+(BR2)SO or HP9+(BR1)Product+(BR1)Product) |
| Reaction74 | SO14+O3**→**(1/6)((BR1)acetone+(BR1)6-MHO+(BR1)Geranylacetone+(BR2)CI1+(BR2)CI2+(BR2)CI3+(BR2)SO or HP3+(BR2)SO or HP8+(BR2)Product+(BR1)Product+(BR1)Product+(BR1)Product) |
| Reaction75 | CISOorHP2+H2O**→**SOorHP2 |
| Reaction76 | CISOorHP2+O3**→**SOorHP2 |
| Reaction77 | CISOorHP2**→**Product |
| Reaction78 | CISOorHP2+allcarbonyl**→**Product |
| Reaction79 | CISOorHP5+H2O**→**SOorHP6 |
| Reaction80 | CISOorHP5+O3**→**SOorHP6 |
| Reaction81 | CISOorHP5**→**Product |
| Reaction82 | CISOorHP5+allcarbonyl**→**Product |
| Reaction83 | SOorHP2+allCI**→**Product |
| Reaction84 | SOorHP3+allCI**→**Product |
| Reaction85 | SOorHP4+allCI**→**Product |
| Reaction86 | SOorHP6+allCI**→**Product |
| Reaction87 | SOorHP7+allCI**→**Product |
| Reaction88 | SOorHP8+allCI**→**Product |
| Reaction89 | SOorHP9+allCI**→**Product |
| Reaction90 | CI1+Acids**→**Product |
| Reaction91 | CI12+Acids**→**SOorHP4 |
| Reaction92 | CI2+Acids**→**SOorHP5 |
| Reaction93 | CI16+Acids**→**SOorHP9 |
| Reaction94 | CI3+Acids**→**SOorHP10 |
| Reaction95 | CI4+Acids**→**SOorHP14 |
| Reaction96 | CI5+Acids**→**Product |
| Reaction97 | CI6+Acids**→**Product |
| Reaction98 | CISOorHP2+Acids**→**Product |
| Reaction99 | CISOorHP5+Acids**→**Product |
| Reaction100 | OtherDB+O3**→**CIDB+Product |
| Reaction101 | CIDB+H2O**→**carbonylproduct |
| Reaction102 | CIDB+O3**→**carbonylproduct |
| Reaction103 | CIDB**→**Acids |
| Reaction104 | CIDB+allcarbonyl**→**Product |
| Reaction105 | Acids+allCI**→**Product |
| Reaction106 | carbonylproduct+allCI**→**Product |

Note that ‘Product’ is not treated in the code.