atom\_par H 2.00 0.020 0.0000 0.00051 0.0 0.0 0 -1 -1 3 H # Non H-bonding Hydrogen

atom\_par HD 2.00 0.020 0.0000 0.00051 0.0 0.0 2 -1 -1 3 H # Donor 1 H-bond Hydrogen

atom\_par HS 2.00 0.020 0.0000 0.00051 0.0 0.0 1 -1 -1 3 H # Donor S Spherical Hydrogen

atom\_par C 4.00 0.150 33.5103 -0.00143 0.0 0.0 0 -1 -1 0 C # Non H-bonding Aliphatic Carbon

atom\_par A 4.00 0.150 33.5103 -0.00052 0.0 0.0 0 -1 -1 0 C # Non H-bonding Aromatic Carbon

atom\_par N 3.50 0.160 22.4493 -0.00162 0.0 0.0 0 -1 -1 1 N # Non H-bonding Nitrogen

atom\_par NA 3.50 0.160 22.4493 -0.00162 1.9 5.0 4 -1 -1 1 N # Acceptor 1 H-bond Nitrogen

atom\_par NS 3.50 0.160 22.4493 -0.00162 1.9 5.0 3 -1 -1 1 N # Acceptor S Spherical Nitrogen

atom\_par OA 3.20 0.200 17.1573 -0.00251 1.9 5.0 5 -1 -1 2 O # Acceptor 2 H-bonds Oxygen

atom\_par OS 3.20 0.200 17.1573 -0.00251 1.9 5.0 3 -1 -1 2 O # Acceptor S Spherical Oxygen

atom\_par F 3.09 0.080 15.4480 -0.00110 0.0 0.0 0 -1 -1 4 F # Non H-bonding Fluorine

atom\_par Mg 1.30 0.875 1.5600 -0.00110 0.0 0.0 0 -1 -1 4 Mg # Non H-bonding Magnesium

atom\_par MG 1.30 0.875 1.5600 -0.00110 0.0 0.0 0 -1 -1 4 Mg # Non H-bonding Magnesium

atom\_par P 4.20 0.200 38.7924 -0.00110 0.0 0.0 0 -1 -1 5 P # Non H-bonding Phosphorus

atom\_par SA 4.00 0.200 33.5103 -0.00214 2.5 1.0 5 -1 -1 6 S # Acceptor 2 H-bonds Sulphur

atom\_par S 4.00 0.200 33.5103 -0.00214 0.0 0.0 0 -1 -1 6 S # Non H-bonding Sulphur

atom\_par Cl 4.09 0.276 35.8235 -0.00110 0.0 0.0 0 -1 -1 4 Cl # Non H-bonding Chlorine

atom\_par CL 4.09 0.276 35.8235 -0.00110 0.0 0.0 0 -1 -1 4 Cl # Non H-bonding Chlorine

atom\_par Ca 1.98 0.550 2.7700 -0.00110 0.0 0.0 0 -1 -1 4 Ca # Non H-bonding Calcium

atom\_par CA 1.98 0.550 2.7700 -0.00110 0.0 0.0 0 -1 -1 4 Ca # Non H-bonding Calcium

atom\_par Mn 1.30 0.875 2.1400 -0.00110 0.0 0.0 0 -1 -1 4 Mn # Non H-bonding Manganese

atom\_par MN 1.30 0.875 2.1400 -0.00110 0.0 0.0 0 -1 -1 4 Mn # Non H-bonding Manganese

atom\_par Fe 1.30 0.010 1.8400 -0.00110 0.0 0.0 0 -1 -1 4 Fe # Non H-bonding Iron

atom\_par FE 1.30 0.010 1.8400 -0.00110 0.0 0.0 0 -1 -1 4 Fe # Non H-bonding Iron

atom\_par Zn 1.48 0.550 1.7000 -0.00110 0.0 0.0 0 -1 -1 4 Zn # Non H-bonding Zinc

atom\_par ZN 1.48 0.550 1.7000 -0.00110 0.0 0.0 0 -1 -1 4 Zn # Non H-bonding Zinc

atom\_par Br 4.33 0.389 42.5661 -0.00110 0.0 0.0 0 -1 -1 4 Br # Non H-bonding Bromine

atom\_par BR 4.33 0.389 42.5661 -0.00110 0.0 0.0 0 -1 -1 4 Br # Non H-bonding Bromine

atom\_par I 4.72 0.550 55.0585 -0.00110 0.0 0.0 0 -1 -1 4 I # Non H-bonding Iodine

atom\_par Z 4.00 0.150 33.5103 -0.00143 0.0 0.0 0 -1 -1 0 D # Non H-bonding covalent map

atom\_par G 4.00 0.150 33.5103 -0.00143 0.0 0.0 0 -1 -1 0 D # Ring closure Glue Aliphatic Carbon # SF

atom\_par GA 4.00 0.150 33.5103 -0.00052 0.0 0.0 0 -1 -1 0 D # Ring closure Glue Aromatic Carbon # SF

atom\_par J 4.00 0.150 33.5103 -0.00143 0.0 0.0 0 -1 -1 0 D # Ring closure Glue Aliphatic Carbon # SF

atom\_par Q 4.00 0.150 33.5103 -0.00143 0.0 0.0 0 -1 -1 0 D # Ring closure Glue Aliphatic Carbon # SF

atom\_par W 0.00 0.200 00.0000 -0.00000 0.0 0.0 0 -1 -1 2 O # Acceptor 2 H-bonds Oxygen