**Table 1: Group Environmental Descriptors used in UPPER (hydrogens implicit)**

**Symbol Description**

x^ Group or atom that is not in an aliphatic ring and is bonded only to sp3 hybrid atoms.

y Group or atom that is not in an aromatic ring and is bonded to one sp2 hybrid atom.

yy Aliphatic atom that is not in a ring and is bonded to two sp2 hybrid atoms.

yyy Aliphatic group or atom that is not in a ring and is bonded to three sp2 hybrid atoms.

yyyy Aliphatic group or atom that is not in a ring and is bonded to four sp2 hybrid atoms.

z Group or atom bonded to a sp hybrid atom.

yz Group bonded to both sp2 and sp hybrid atoms.

a atom in an aromatic ring and is bonded to one sp3 hybrid atom.

aa Atom in an aromatic ring and is between two aromatic rings.

aaa Atom in an aromatic ring and is between three aromatic rings.

ay Atom in an aromatic ring and is bonded to one sp2 hybrid atom that is not in an aromatic ring.

az Atom in an aromatic ring and is bonded to one sp hybrid atom.

bip Atom in the 2 or 6 position in biphenyl.

r Atom in an aliphatic ring.

rr Atom contained between two fused aliphatic rings.

ar Atom contained between one aromatic and one aliphatic fused ring system.

ary Atom contained between one aromatic and one aliphatic fused ring system and bonded to sp2 hybrid atom that is not in an aromatic ring.

arr Atom contained between one aromatic and two aliphatic fused rings system.

ry Atom in an aliphatic ring not part of a fused ring system and bonded to one sp2 hybrid atom.

rz Atom in an aliphatic ring not part of a fused ring system and bonded to one sp hybrid atom.

ryy Atom in an aliphatic ring not part of a fused ring system and bonded to two sp2 hybrid atoms.

rry Atom contained between two aliphatic rings and bonded to one sp2 hybrid atom.

rrz Atom contained between two aliphatic rings and bonded to one sp hybrid atom.

rryy Atom contained between two aliphatic rings and bonded to two sp2 hybrid atoms.

rryz Atom contained between two aliphatic rings and bonded to one sp2 and one sp hybrid atoms.

rryyy Atom contained between two aliphatic rings and bonded to three sp2 hybrid atoms.

rrr Atom contained between three fused aliphatic rings.

= Double bond in the group or for terminal sp2 group.

# Triple bond in the group or for terminal sp group.

rC= Atom in an aliphatic ring not part of a fused ring system and contains double bond inside of aliphatic ring.

rC=\* Atom in an aliphatic ring not part of a fused ring system and contains double bond outside of aliphatic ring. \* Denotes any atom.

rrC= Atom between 2 fused aliphatic rings and contains double bond.

rryC= Atom between 2 fused aliphatic rings, contains double bond, and is bonded to one sp2 hybrid atom.

rryyC= Atom between 2 fused aliphatic rings, contains double bond, and is bonded to two sp2 hybrid atoms.

^the x can be left out if the group is obviously aliphatic