





## Bond types:

- : Single  
= : Double  
T : Triple  
# : Triple  
~ : Single or double query bond  
% : An aromatic query bond

None : Any bond type; no explicit bond specified

\$ : Ring bond; \$ before a bond type specifies ring bond  
! : Chain or non-ring bond; ! before a bond type specifies chain bond

@ : A ring linkage and the number following it specifies the atoms position in the line, thus @1 means linked back to the first atom in the list.

Aromatic: Kekule or Arom5

Kekule: Bonds in 6-membered rings with alternate single/double bonds or perimeter bonds  
Arom5: Bonds in 5-membered rings with two double bonds and a hetro atom at the apex of the ring.

MACCS 166 keys [ Ref 45-47 ] are defined as follows:

## Key Description

1 ISOTOPE  
2 103 < ATOMIC NO. < 256  
3 GROUP IVA,VA,VIA PERIODS 4-6 (Ge...)  
4 ACTINIDE  
5 GROUP IIIB,IVB (Sc...)  
6 LANTHANIDE  
7 GROUP VB,VIB,VIIB (V...)  
8 QAAA@1  
9 GROUP VIII (Fe...)  
10 GROUP IIA (ALKALINE EARTH)  
11 4M RING  
12 GROUP IB,IIB (Cu...)  
13 ON(C)C  
14 S-S  
15 OC(O)O  
16 QAA@1  
17 CTC  
18 GROUP IIIA (B...)  
19 7M RING  
20 SI  
21 C=C(Q)Q  
22 3M RING  
23 NC(O)O  
24 N-O  
25 NC(N)N  
26 C\$=C(\$A)\$A  
27 I  
28 QCH2Q  
29 P  
30 CQ(C)(C)A  
31 QX  
32 CSN  
33 NS  
34 CH2=A  
35 GROUP IA (ALKALI METAL)  
36 S HETEROCYCLE  
37 NC(O)N  
38 NC(C)N  
39 OS(O)O  
40 S-O

41 CTN  
42 F  
43 QHAQH  
44 OTHER  
45 C=CN  
46 BR  
47 SAN  
48 OQ(O)O  
49 CHARGE  
50 C=C(C)C  
51 CSO  
52 NN  
53 QHAAAQH  
54 QHAAQH  
55 OSO  
56 ON(O)C  
57 O HETEROCYCLE  
58 QSQ  
59 Snot%A%A  
60 S=O  
61 AS(A)A  
62 A\$A!A\$A  
63 N=O  
64 A\$A!S  
65 C%N  
66 CC(C)(C)A  
67 QS  
68 QHQH (&...)  
69 QQH  
70 QNQ  
71 NO  
72 OAAO  
73 S=A  
74 CH3ACH3  
75 A!N\$A  
76 C=C(A)A  
77 NAN  
78 C=N  
79 NAAAN  
80 NAAAN  
81 SA(A)A  
82 ACH2QH  
83 QAAAA@1  
84 NH2  
85 CN(C)C  
86 CH2QCH2  
87 X!A\$A  
88 S  
89 OAAAO  
90 QHAACH2A  
91 QHAAACH2A  
92 OC(N)C  
93 QCH3  
94 QN  
95 NAAO  
96 5M RING  
97 NAAAO  
98 QAAAAA@1  
99 C=C  
100 ACH2N  
101 8M RING  
102 QO  
103 CL  
104 QHACH2A  
105 A\$A(\$A)\$A  
106 QA(Q)Q  
107 XA(A)A  
108 CH3AAACH2A  
109 ACH2O

110 NCO  
111 NACH2A  
112 AA(A)(A)A  
113 Onot%A%A  
114 CH3CH2A  
115 CH3ACH2A  
116 CH3AACH2A  
117 NAO  
118 ACH2CH2A > 1  
119 N=A  
120 HETEROCYCLIC ATOM > 1 (&...)  
121 N HETEROCYCLE  
122 AN(A)A  
123 OCO  
124 QQ  
125 AROMATIC RING > 1  
126 A!O!A  
127 A\$A!O > 1 (&...)  
128 ACH2AAACH2A  
129 ACH2AACH2A  
130 QQ > 1 (&...)  
131 QH > 1  
132 OACH2A  
133 A\$A!N  
134 X (HALOGEN)  
135 Nnot%A%A  
136 O=A > 1  
137 HETEROCYCLE  
138 QCH2A > 1 (&...)  
139 OH  
140 O > 3 (&...)  
141 CH3 > 2 (&...)  
142 N > 1  
143 A\$A!O  
144 Anot%A%Anot%A  
145 6M RING > 1  
146 O > 2  
147 ACH2CH2A  
148 AQ(A)A  
149 CH3 > 1  
150 A!A\$A!A  
151 NH  
152 OC(C)C  
153 QCH2A  
154 C=O  
155 A!CH2!A  
156 NA(A)A  
157 C-O  
158 C-N  
159 O > 1  
160 CH3  
161 N  
162 AROMATIC  
163 6M RING  
164 O  
165 RING  
166 FRAGMENTS

MACCS 322 keys set as defined in tables 1, 2 and 3 [ Ref 46 ] include:

- o 26 atom properties of type P, as listed in Table 1
- o 32 one-atom environments, as listed in Table 3
- o 264 atom-bond-atom combinations listed in Table 4

Total number of keys in three tables is : 322

Atom symbol, X, used for 322 keys [ Ref 46 ] doesn't refer to Halogens as it does for 166 keys. In order to keep the definition of 322 keys consistent with the published definitions, the symbol X is used to imply "others" atoms, but it's internally mapped to symbol X as defined for 166 keys during the generation of key values.

## Atom properties-based keys (26):

| Key | Description   |
|-----|---|
| 1   | A(AAA) or AA(A)A - atom with at least three neighbors   |
| 2   | Q - heteroatom  |
| 3   | Anot%not-A - atom involved in one or more multiple bonds, not aromatic  |
| 4   | A(AAAA) or AA(A)(A)A - atom with at least four neighbors  |
| 5   | A(QQ) or QA(Q) - atom with at least two heteroatom neighbors  |
| 6   | A(QQQ) or QA(Q)Q - atom with at least three heteroatom neighbors  |
| 7   | QH - heteroatom with at least one hydrogen attached   |
| 8   | CH2(AA) or ACH2A - carbon with at least two single bonds and at least two hydrogens attached  |
| 9   | CH3(A) or ACH3 - carbon with at least one single bond and at least three hydrogens attached   |
| 10  | Halogen   |
| 11  | A(-A-A-A) or A-A(-A)-A - atom has at least three single bonds   |
| 12  | AAAAA@1 > 2 - atom is in at least two different six-membered rings  |
| 13  | A(\$A\$A\$A) or A\$A(\$A)\$A - atom has more than two ring bonds  |
| 14  | A\$A!A\$A - atom is at a ring/chain boundary. When a comparison is done with another atom the path passes through the chain bond.                   |
| 15  | Anot%A%not%A - atom is at an aromatic/nonaromatic boundary. When a comparison is done with another atom the path passes through the aromatic bond.  |
| 16  | A!A!A - atom with more than one chain bond  |
| 17  | A!A\$A!A - atom is at a ring/chain boundary. When a comparison is done with another atom the path passes through the ring bond.                     |
| 18  | A%Anot%A%A - atom is at an aromatic/nonaromatic boundary. When a comparison is done with another atom the path passes through the nonaromatic bond. |
| 19  | HETEROCYCLE - atom is a heteroatom in a ring.   |
| 20  | rare properties: atom with five or more neighbors, atom in four or more rings, or atom types other than H, C, N, O, S, F, Cl, Br, or I              |
| 21  | rare properties: atom has a charge, is an isotope, has two or more multiple bonds, or has a triple bond.  |
| 22  | N - nitrogen  |
| 23  | S - sulfur  |
| 24  | O - oxygen  |
| 25  | A(AA)A(A)A(AA) - atom has two neighbors, each with three or more neighbors (including the central atom).  |
| 26  | CHACH2 - atom has two hydrocarbon (CH2) neighbors   |

## Atomic environments properties-based keys (32):

| Key | Description |
|-----|-------------|
| 27  | C(CC)       |
| 28  | C(CCC)      |
| 29  | C(CN)       |
| 30  | C(CCN)      |
| 31  | C(NN)       |
| 32  | C(NNC)      |
| 33  | C(NNN)      |
| 34  | C(CO)       |
| 35  | C(CCO)      |
| 36  | C(NO)       |
| 37  | C(NCO)      |
| 38  | C(NNO)      |
| 39  | C(OO)       |
| 40  | C(COO)      |
| 41  | C(NOO)      |
| 42  | C(OOO)      |
| 43  | Q(CC)       |
| 44  | Q(CCC)      |
| 45  | Q(CN)       |
| 46  | Q(CCN)      |
| 47  | Q(NN)       |
| 48  | Q(CNN)      |
| 49  | Q(NNN)      |
| 50  | Q(CO)       |
| 51  | Q(CCO)      |

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|    |        |
|----|--------|
| 52 | Q(NO)  |
| 53 | Q(CNO) |
| 54 | Q(NNO) |
| 55 | Q(OO)  |
| 56 | Q(COO) |
| 57 | Q(NOO) |
| 58 | Q(OOO) |

Note: The first symbol is the central atom, with atoms bonded to the central atom listed in parentheses. Q is any non-C, non-H atom. If only two atoms are in parentheses, there is no implication concerning the other atoms bonded to the central atom.

Atom-Bond-Atom properties-based keys: (264)

| Key | Description |
|-----|-------------|
| 59  | C-C         |
| 60  | C-N         |
| 61  | C-O         |
| 62  | C-S         |
| 63  | C-Cl        |
| 64  | C-P         |
| 65  | C-F         |
| 66  | C-Br        |
| 67  | C-Si        |
| 68  | C-I         |
| 69  | C-X         |
| 70  | N-N         |
| 71  | N-O         |
| 72  | N-S         |
| 73  | N-Cl        |
| 74  | N-P         |
| 75  | N-F         |
| 76  | N-Br        |
| 77  | N-Si        |
| 78  | N-I         |
| 79  | N-X         |
| 80  | O-O         |
| 81  | O-S         |
| 82  | O-Cl        |
| 83  | O-P         |
| 84  | O-F         |
| 85  | O-Br        |
| 86  | O-Si        |
| 87  | O-I         |
| 88  | O-X         |
| 89  | S-S         |
| 90  | S-Cl        |
| 91  | S-P         |
| 92  | S-F         |
| 93  | S-Br        |
| 94  | S-Si        |
| 95  | S-I         |
| 96  | S-X         |
| 97  | Cl-Cl       |
| 98  | Cl-P        |
| 99  | Cl-F        |
| 100 | Cl-Br       |
| 101 | Cl-Si       |
| 102 | Cl-I        |
| 103 | Cl-X        |
| 104 | P-P         |
| 105 | P-F         |
| 106 | P-Br        |
| 107 | P-Si        |
| 108 | P-I         |
| 109 | P-X         |
| 110 | F-F         |
| 111 | F-Br        |
| 112 | F-Si        |
| 113 | F-I         |

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|     |       |
|-----|-------|
| 114 | F-X   |
| 115 | Br-Br |
| 116 | Br-Si |
| 117 | Br-I  |
| 118 | Br-X  |
| 119 | Si-Si |
| 120 | Si-I  |
| 121 | Si-X  |
| 122 | I-I   |
| 123 | I-X   |
| 124 | X-X   |
| 125 | C=C   |
| 126 | C=N   |
| 127 | C=O   |
| 128 | C=S   |
| 129 | C=Cl  |
| 130 | C=P   |
| 131 | C=F   |
| 132 | C=Br  |
| 133 | C=Si  |
| 134 | C=I   |
| 135 | C=X   |
| 136 | N=N   |
| 137 | N=O   |
| 138 | N=S   |
| 139 | N=Cl  |
| 140 | N=P   |
| 141 | N=F   |
| 142 | N=Br  |
| 143 | N=Si  |
| 144 | N=I   |
| 145 | N=X   |
| 146 | O=O   |
| 147 | O=S   |
| 148 | O=Cl  |
| 149 | O=P   |
| 150 | O=F   |
| 151 | O=Br  |
| 152 | O=Si  |
| 153 | O=I   |
| 154 | O=X   |
| 155 | S=S   |
| 156 | S=Cl  |
| 157 | S=P   |
| 158 | S=F   |
| 159 | S=Br  |
| 160 | S=Si  |
| 161 | S=I   |
| 162 | S=X   |
| 163 | Cl=Cl |
| 164 | Cl=P  |
| 165 | Cl=F  |
| 166 | Cl=Br |
| 167 | Cl=Si |
| 168 | Cl=I  |
| 169 | Cl=X  |
| 170 | P=P   |
| 171 | P=F   |
| 172 | P=Br  |
| 173 | P=Si  |
| 174 | P=I   |
| 175 | P=X   |
| 176 | F=F   |
| 177 | F=Br  |
| 178 | F=Si  |
| 179 | F=I   |
| 180 | F=X   |
| 181 | Br=Br |
| 182 | Br=Si |

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|     |       |
|-----|-------|
| 183 | Br=I  |
| 184 | Br=X  |
| 185 | Si=Si |
| 186 | Si=I  |
| 187 | Si=X  |
| 188 | I=I   |
| 189 | I=X   |
| 190 | X=X   |
| 191 | C#C   |
| 192 | C#N   |
| 193 | C#O   |
| 194 | C#S   |
| 195 | C#Cl  |
| 196 | C#P   |
| 197 | C#F   |
| 198 | C#Br  |
| 199 | C#Si  |
| 200 | C#I   |
| 201 | C#X   |
| 202 | N#N   |
| 203 | N#O   |
| 204 | N#S   |
| 205 | N#Cl  |
| 206 | N#P   |
| 207 | N#F   |
| 208 | N#Br  |
| 209 | N#Si  |
| 210 | N#I   |
| 211 | N#X   |
| 212 | O#O   |
| 213 | O#S   |
| 214 | O#Cl  |
| 215 | O#P   |
| 216 | O#F   |
| 217 | O#Br  |
| 218 | O#Si  |
| 219 | O#I   |
| 220 | O#X   |
| 221 | S#S   |
| 222 | S#Cl  |
| 223 | S#P   |
| 224 | S#F   |
| 225 | S#Br  |
| 226 | S#Si  |
| 227 | S#I   |
| 228 | S#X   |
| 229 | Cl#Cl |
| 230 | Cl#P  |
| 231 | Cl#F  |
| 232 | Cl#Br |
| 233 | Cl#Si |
| 234 | Cl#I  |
| 235 | Cl#X  |
| 236 | P#P   |
| 237 | P#F   |
| 238 | P#Br  |
| 239 | P#Si  |
| 240 | P#I   |
| 241 | P#X   |
| 242 | F#F   |
| 243 | F#Br  |
| 244 | F#Si  |
| 245 | F#I   |
| 246 | F#X   |
| 247 | Br#Br |
| 248 | Br#Si |
| 249 | Br#I  |
| 250 | Br#X  |
| 251 | Si#Si |

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|     |        |
|-----|--------|
| 252 | Si#I   |
| 253 | Si#X   |
| 254 | I#I    |
| 255 | I#X    |
| 256 | X#X    |
| 257 | C\$C   |
| 258 | C\$N   |
| 259 | C\$O   |
| 260 | C\$S   |
| 261 | C\$Cl  |
| 262 | C\$P   |
| 263 | C\$F   |
| 264 | C\$Br  |
| 265 | C\$Si  |
| 266 | C\$I   |
| 267 | C\$X   |
| 268 | N\$N   |
| 269 | N\$O   |
| 270 | N\$S   |
| 271 | N\$Cl  |
| 272 | N\$P   |
| 273 | N\$F   |
| 274 | N\$Br  |
| 275 | N\$Si  |
| 276 | N\$I   |
| 277 | N\$X   |
| 278 | O\$O   |
| 279 | O\$S   |
| 280 | O\$Cl  |
| 281 | O\$P   |
| 282 | O\$F   |
| 283 | O\$Br  |
| 284 | O\$Si  |
| 285 | O\$I   |
| 286 | O\$X   |
| 287 | S\$S   |
| 288 | S\$Cl  |
| 289 | S\$P   |
| 290 | S\$F   |
| 291 | S\$Br  |
| 292 | S\$Si  |
| 293 | S\$I   |
| 294 | S\$X   |
| 295 | Cl\$Cl |
| 296 | Cl\$P  |
| 297 | Cl\$F  |
| 298 | Cl\$Br |
| 299 | Cl\$Si |
| 300 | Cl\$I  |
| 301 | Cl\$X  |
| 302 | P\$P   |
| 303 | P\$F   |
| 304 | P\$Br  |
| 305 | P\$Si  |
| 306 | P\$I   |
| 307 | P\$X   |
| 308 | F\$F   |
| 309 | F\$Br  |
| 310 | F\$Si  |
| 311 | F\$I   |
| 312 | F\$X   |
| 313 | Br\$Br |
| 314 | Br\$Si |
| 315 | Br\$I  |
| 316 | Br\$X  |
| 317 | Si\$Si |
| 318 | Si\$I  |
| 319 | Si\$X  |
| 320 | I\$I   |

---

```
321  I$X
322  X$X
```

#### SetSize

```
$MACCSKeys->SetSize($Size);
```

Sets size of MACCS keys and returns *MACCSKeys*. Possible values: *166* or *322*.

#### SetType

```
$MACCSKeys->SetType($Type);
```

Sets type of MACCS keys and returns *MACCSKeys*. Possible values: *MACCSKeysBits* or *MACCSKeysCount*.

#### StringifyMACCSKeys

```
$String = $MACCSKeys->StringifyMACCSKeys();
```

Returns a string containing information about *MACCSKeys* object.

#### AUTHOR

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#### SEE ALSO

Fingerprints.pm, FingerprintsStringUtil.pm, AtomNeighborhoodsFingerprints.pm, AtomTypesFingerprints.pm, EStateIndicesFingerprints.pm, ExtendedConnectivityFingerprints.pm, PathLengthFingerprints.pm, TopologicalAtomPairsFingerprints.pm, TopologicalAtomTripletsFingerprints.pm, TopologicalAtomTorsionsFingerprints.pm, TopologicalPharmacophoreAtomPairsFingerprints.pm, TopologicalPharmacophoreAtomTripletsFingerprints.pm

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