iii. Filename “extra_pts.f” in the SANDER subprogram to increase the number of lone-pairs per molecule and treat LP identically to EP

Original file

line 122
```
integer ep,blank,n,max14
```

line 129
```
max14 = 12*(nphih+nphia+ndper)
```

lines 160-161
```
integer ep,blank,n,numextra_test
data ep/4HEP  /
```

line 172
```
 if ( isymbl(n) .eq. ep )then
```

line 209
```
+    natom,isymbl,ep,
```

line 286
```
+    numatoms,isymbl,ep,
```

line 291
```
+    isymbl(*),numatoms,ep
```

line 311
```
 if ( isymbl(ii) .eq. ep ) then
```

line 316
```
 else if ( isymbl(jj) .eq. ep ) then
```

Modified file

line 122
```
integer ep,lp,blank,n,max14
```

line 129
```
max14 = 24*(nphih+nphia+ndper)
```

lines 160-161
```
integer ep,lp,blank,n,numextra_test
data ep/4HEP  /, lp/4HLP  /
```

line 172
```
 if ((isymbl(n) .eq. ep) .or. (isymbl(n) .eq. lp))then
```

line 209
```
+    natom,isymbl,ep,lp,
```

line 286
```
+    numatoms,isymbl,ep,lp,
```

line 291
```
+    isymbl(*),numatoms,ep,lp
```

line 311
```
 if (( isymbl(ii) .eq. ep) .or. ( isymbl(ii) .eq. lp)) then
```

line 316
```
 else if (( isymbl(jj).eq.ep).or.(isymbl(jj) .eq. lp)) then
```