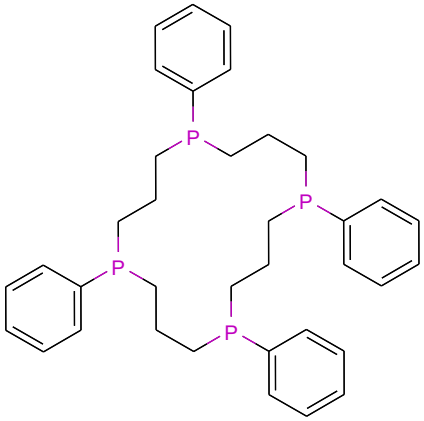
```
using BenchmarkTools    , MolecularGraph
```

```
mol1 =
```

```
GraphMol([Dict(44 => 40, 8 => 8, 1 => 2), Dict(7 => 7, 2 => 3, 1 => 1), Dict(2 => 2, 3 =>
```

```
mol1 = smilestomol("P1(c2ccccc2)CCCP(c3ccccc3)CCCP(c4ccccc4)CCCP(c5ccccc5)CCC1")
```




```
HTML(drawsvg(mol1, 250, 250))
```

```
access_arom_from_struct (generic function with 1 method)
```

```
function access_arom_from_struct(mol::GraphMol)::Vector{Bool}
    return [bond.isaromatic for bond in mol.edgeattrs]
end
```

```
[false, false, false, false, false, false, false, false, false, false, false, false, false,
```

```
@btime access_arom_from_struct(mol1)
```

```
  66.191 ns (1 allocation: 96 bytes)
```

```
BitVector: [false, true, true, true, true, true, true, false, false, false, false, false, t
```

```
@btime isaromaticbond(mol1)
```

```
  3.954 ms (20117 allocations: 4.93 MiB)
```

```
begin
    mol1a = deepcopy(mol1)
    precalculate!(mol1a)
end;
```

```
BitVector: [false, true, true, true, true, true, true, false, false, false, false, false, t
```

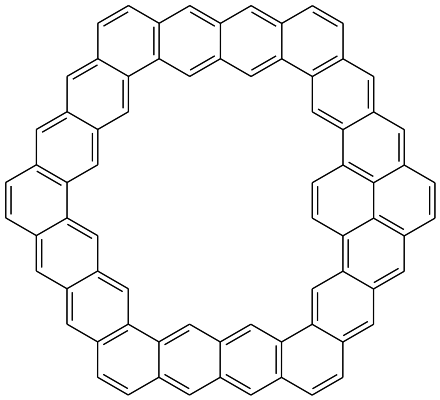
```
@btime isaromaticbond(mol1a)
```

```
3.300 μs (79 allocations: 6.86 KiB)
```

mol2 =

```
GraphMol([Dict(93 => 74, 3 => 4, 1 => 2), Dict(2 => 3, 1 => 1), Dict(2 => 2, 38 => 36), Di
```

```
mol2 =
smilestomol("C1(C=C2)=C3C=C(C=C(C(C=C(C=C(C=C(C(C(C=C(C=C(C(C=C(C=C(C(C=C(C(C=C4)=C(C(C4=C(C
=C3C2=C5)C5=C6)=C6C=C7)C7=C8)C8=C9)=C9C=C%10)C%10=C%11)C%11=C%12)=C%12C=C%13)C%13=C%14
)C%14=C%15)=C%15C=C%16)C%16=C%17)C%17=C%18)=C%18C=C%19)C%19=C%20)C%20=C1")
```



```
HTML(drawsvg(mol2, 250, 250))
```

```
[false, false, false, false, false, false, false, false, false, false, false, false, false,
```

```
@btime access_arom_from_struct(mol2)
```

```
97.484 ns (1 allocation: 144 bytes)
```

```
BitVector: [true, true, true, true, true, true, true, true, true, true, true, true, true, t
```

```
@btime isaromaticbond(mol2)
```

```
55.346 ms (136800 allocations: 44.28 MiB)
```

```
begin
    mol2a = deepcopy(mol2)
    precalculate!(mol2a)
end;
```

```
BitVector: [true, true, true, true, true, true, true, true, true, true, true, true, true, t
```

```
@btime isaromaticbond(mol2a)
```

```
  18.100 μs (389 allocations: 36.09 KiB)
```