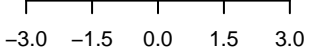
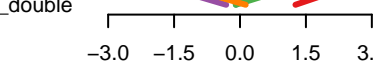


Adjacency, distance matrix, connectivity, Kappa shape in



EIL,5,6014) Atom and bond col
 a_aro
 a_nB
 a_nH
 a_nS
 double



(EII,5,6014) Atom and bond counts

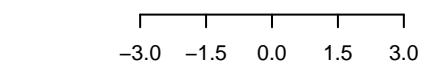
b_heavy

chiral

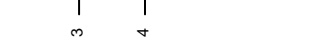
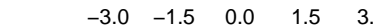
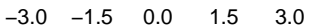
_violation

opr_nrot

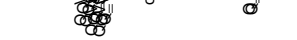
VDistMa



(EII,5,6014) Partial charge



```
dist(avg_p)
hclust (*, "complete")
```



```
dist(t(avg_p))
hclust (*, "complete")
```