# SI Electronegativity project

**cph\_res  
*E*** = –344.00 kcal mol–1***H*** = –333.31 kcal mol–1***G*** = –348.62 kcal mol–1Nimag = 0

C -0.08005188 0.00758745 0.00000000  
H 0.99604332 0.05963580 0.00000000  
P -1.62599148 -0.06722326 0.00000000

**cash\_res  
*E*** = –315.50 kcal mol–1***H*** = –305.31 kcal mol–1***G*** = –321.49 kcal mol–1Nimag = 0

C 0.19455386 0.00877475 0.00000000  
H 1.27303066 0.05749767 0.00000000  
As -1.46758452 -0.06627244 0.00000000

**csbh\_res  
*E*** = –283.62 kcal mol–1***H*** = –273.83 kcal mol–1***G*** = –290.62 kcal mol–1Nimag = 0

C 0.19555334 0.01071896 0.00000000  
H 1.27848831 0.05496651 0.00000000  
Sb -1.67404167 -0.06568549 0.00000000

**None**

**cnh\_temp  
*E*** = –440.02 kcal mol–1***H*** = –427.63 kcal mol–1***G*** = –444.33 kcal mol–1Nimag = 0

C 0.02799864 0.00186306 0.00000000  
H 1.09787678 0.07189137 0.00000000  
N -1.12587542 -0.07375444 0.00000000

**None**

**cteh2\_res  
*E*** = –375.90 kcal mol–1***H*** = –359.18 kcal mol–1***G*** = –377.13 kcal mol–1Nimag = 0

C -0.23470374 0.00000000 0.00000000  
Te 1.74599753 0.00000000 0.00000000  
H -0.80564690 -0.92675028 0.00000000  
H -0.80564690 0.92675028 0.00000000

**csh2\_res  
*E*** = –420.08 kcal mol–1***H*** = –402.66 kcal mol–1***G*** = –419.12 kcal mol–1Nimag = 0

C -0.13905976 0.00000000 0.00000000  
S 1.48258150 0.00000000 0.00000000  
H -0.72176088 -0.92660946 0.00000000  
H -0.72176088 0.92660946 0.00000000

**coh2\_res  
*E*** = –494.36 kcal mol–1***H*** = –475.92 kcal mol–1***G*** = –491.51 kcal mol–1Nimag = 0

C -0.03257591 0.00000000 0.00000000  
O 1.17922521 0.00000000 0.00000000  
H -0.62332465 -0.94517944 0.00000000  
H -0.62332465 0.94517944 0.00000000

**cseh2\_res  
*E*** = –397.74 kcal mol–1***H*** = –380.68 kcal mol–1***G*** = –398.03 kcal mol–1Nimag = 0

C -0.18140400 0.00000000 0.00000000  
Se 1.58926207 0.00000000 0.00000000  
H -0.75392904 -0.92820667 0.00000000  
H -0.75392904 0.92820667 0.00000000

**cclh3\_res  
*E*** = –494.72 kcal mol–1***H*** = –469.25 kcal mol–1***G*** = –486.63 kcal mol–1Nimag = 0

C -0.10793171 -0.00001234 0.00000000  
Cl 1.71309929 0.00006194 0.00000000  
H -0.44408591 1.03737809 0.00000000  
H -0.44404083 -0.51871384 0.89841485  
H -0.44404083 -0.51871384 -0.89841485

**cih3\_res  
*E*** = –470.81 kcal mol–1***H*** = –445.93 kcal mol–1***G*** = –464.73 kcal mol–1Nimag = 0

C -0.19272177 -0.00002711 0.00000000  
I 1.99677052 0.00023967 0.00000000  
H -0.51050420 1.04082532 0.00000000  
H -0.51027226 -0.52051894 0.90144780  
H -0.51027226 -0.52051894 -0.90144780

**cfh3\_res  
*E*** = –534.85 kcal mol–1***H*** = –508.61 kcal mol–1***G*** = –525.17 kcal mol–1Nimag = 0

C -0.01977458 0.00000150 0.00000000  
F 1.39374342 0.00000170 0.00000000  
H -0.36698291 1.03917235 0.00000000  
H -0.36699296 -0.51958777 0.89995225  
H -0.36699296 -0.51958777 -0.89995225

**None**

**None**

**cbrh3\_res  
*E*** = –482.56 kcal mol–1***H*** = –457.40 kcal mol–1***G*** = –475.62 kcal mol–1Nimag = 0

C -0.15002532 -0.00000707 0.00000000  
Br 1.83779006 -0.00000879 0.00000000  
H -0.47157027 1.04022253 0.00000000  
H -0.47159722 -0.52010333 0.90086192  
H -0.47159722 -0.52010333 -0.90086192