Electronic Supplementary Information for Dalton Transactions

DFT B3LYP/6-31G* calculated coordinates for *arachno*-$PhCB_8H_{13}$ (compound 3) and *nido*-$PhCB_8H_{11}$ (compound 4)

Cartesian coordinates for *arachno*-$PhCB_8H_{13}$ (compound 3)

```
0 1
 C    -0.040998     1.648355    -0.636372
 B     1.441622     0.881215    -0.161997
 B     1.635726    -0.894161    -0.589550
 B     0.977275    -0.479973     0.947673
 B     0.080119    -1.650696    -0.069290
 B    -1.677364    -0.955737    -0.585904
 B    -1.464439     0.867926    -0.054917
 B    -0.830575    -0.544126     0.927816
 B     0.011941     0.980064     0.892329
 C    -0.032344     3.097821    -0.597982
 H    -1.269206    -1.403906    -1.629599
 H    -2.737554    -1.410449    -0.292459
 H     0.068060    -2.833045     0.022089
 H    -1.375390    -0.918614     1.913870
 H    -0.069909     1.295048    -1.662451
 H    -2.391608     1.511010     0.313509
 H    -1.858795     0.240638    -1.137215
 H     1.551385    -0.760933     1.948076
 H     0.720888    -1.433549    -1.299828
 H     2.658563    -1.476105    -0.738376
 H     2.406760     1.547498     0.017518
 H     1.695309     0.189713    -1.302521
 H     0.010484     1.806413     1.742447
 C    -0.072594     3.829907    -1.790638
 C    -0.064239     5.229392    -1.753572
 C    -0.015634     5.896790    -0.523849
 C     0.024615     5.164703     0.668807
 C     0.016260     3.765219     0.631741
 H    -0.110401     3.310767    -2.747187
 H    -0.095547     5.798851    -2.681288
 H    -0.009135     6.985388    -0.495017
 H     0.062423     5.683843     1.625356
 H     0.047568     3.195760     1.559457
```

+*x*,*y*,*z*, coordinates for *arachno*-$PhCB_8H_{13}$ (compound 3)

```
33
C 0.145169 0.292363 0.320019
B 0.967865 -1.108464 0.930389
B 2.684680 -0.868919 1.536690
B 2.443172 -1.323933 -0.107329
B 3.487636 0.091054 0.234139
B 2.730603 1.739262 -0.506751
B 0.979385 1.112609 -0.946719
B 2.496128 0.114904 -1.202672
B 0.981644 -0.637671 -0.785282
C -1.290691 0.155836 0.171131
H 3.060283 2.091017 0.599742
H 3.210455 2.426531 -1.351901
H 4.672683 0.131122 0.256568
H 2.976722 -0.033757 -2.277985
H 0.380508 0.970143 1.134714
H 0.377515 1.568856 -1.862431
H 1.478898 2.132372 -0.290254
H 2.837743 -2.368332 -0.510928
H 3.136296 0.325678 1.573345
H 3.250988 -1.539544 2.334538
H 0.330615 -2.026474 1.328914
H 1.527689 -0.558012 2.038057
H 0.256314 -1.218325 -1.521688
C -2.152642 0.865164 1.016053
C -3.538989 0.733345 0.872299
C -4.063386 -0.107802 -0.116377
C -3.201434 -0.817130 -0.961299
C -1.815087 -0.685311 -0.817546
H -1.744737 1.519456 1.785102
H -4.209465 1.285101 1.529528
H -5.141765 -0.210338 -0.228197
H -3.609339 -1.471423 -1.730348
H -1.144612 -1.237066 -1.474775
```

Cartesian coordinates for *nido*-$PhCB_8H_{11}$ (compound 4)

```
0 1
 C    -1.643010     0.000000     0.166666
 B    -0.910877     0.974736    -0.878116
 B     0.769091     1.383009    -0.188835
 B    -0.536097     0.909848     0.902844
 B    -0.536097    -0.909848     0.902844
 B     0.769091    -1.383009    -0.188835
 B    -0.910877    -0.974736    -0.878116
 B     1.007237     0.000000     0.983473
 B     1.909773     0.000000    -0.452185
 H    -0.391759     0.000000    -1.626933
 H     1.599936     0.000000     1.964320
 H     3.057798     0.000000    -0.505452
 H    -1.514305    -1.702684    -1.531591
 H     1.185210    -2.441205    -0.020117
 H    -0.850370    -1.705179     1.671492
 H     1.415568    -0.927863    -1.253908
 H    -1.514305     1.702684    -1.531591
 H     1.185210     2.441205    -0.020117
 H    -0.850371     1.705179     1.671492
 H     1.415568     0.927863    -1.253908
 C    -3.056579     0.000000     0.489656
 C    -4.009064     0.000000    -0.536392
 C    -5.373889     0.000000    -0.224540
 C    -5.786230     0.000000     1.113360
 C    -4.833746     0.000000     2.139407
 C    -3.468920     0.000000     1.827555
 H    -3.688321     0.000000    -1.577087
 H    -6.114786     0.000000    -1.022658
 H    -6.847869     0.000000     1.355936
 H    -5.154488     0.000000     3.180102
 H    -2.728023     0.000000     2.625673
```

+*x*,*y*,*z*, coordinates for *nido*-$PhCB_8H_{11}$ (compound 4)

```
31
C -0.000537 -0.265645 0.000000
B 0.331150 -1.497543 0.974736
B -1.275399 -2.343947 1.383009
B -1.275399 -0.642395 0.909848
B -1.275399 -0.642395 -0.909848
B -1.275399 -2.343947 -1.383009
B 0.331150 -1.497543 -0.974736
B -2.327416 -1.774491 0.000000
B -1.805231 -3.387875 0.000000
H 0.572481 -2.376161 0.000000
H -3.460045 -1.599835 0.000000
H -2.500921 -4.302651 0.000000
H 1.219550 -1.453935 -1.702684
```

H -1.671788 -2.554888 -2.441205
H -1.663365 0.091818 -1.705179
H -0.873193 -3.523160 -0.927863
H 1.219550 -1.453935 1.702684
H -1.671788 -2.554888 2.441205
H -1.663365 0.091818 1.705179
H -0.873193 -3.523160 0.927863
C 0.658627 1.025867 0.000000
C 2.056758 1.098187 0.000000
C 2.693192 2.345164 0.000000
C 1.931495 3.519821 0.000000
C 0.533365 3.447501 0.000000
C -0.103069 2.200523 0.000000
H 2.649249 0.184471 0.000000
H 3.780738 2.401419 0.000000
H 2.426550 4.489790 0.000000
H -0.059127 4.361216 0.000000
H -1.190615 2.144268 0.000000