## Supporting information for

# Synthesis, Characterization, Physical Properties, and OLED Application of Single BN-Fused PeryleneDiimide

Gang Li,[a,b] Yongbiao Zhao,[c] Junbo Li,[a] Jun Cao,[d] Jia Zhu,[d] Xiaowei Sun,[c]* Qichun Zhang [a]*

[a]School of Materials Science Engineering, Nanyang Technological University, 639798, Singapore, E-mail: QCZhang@ntu.edu.sg

[b]Beijing National Laboratory for Molecular Sciences (BNLMS), Institute of Chemistry, ChineseAcademy of Sciences, Beijing, P. R. China

[c]School of Electrical and Electronic Engineering, Nanyang Technological University, 639798, Singapore, E-mail: EXWSun@ntu.edu.sg

[d]Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, 100875 Beijing, China

## Contents

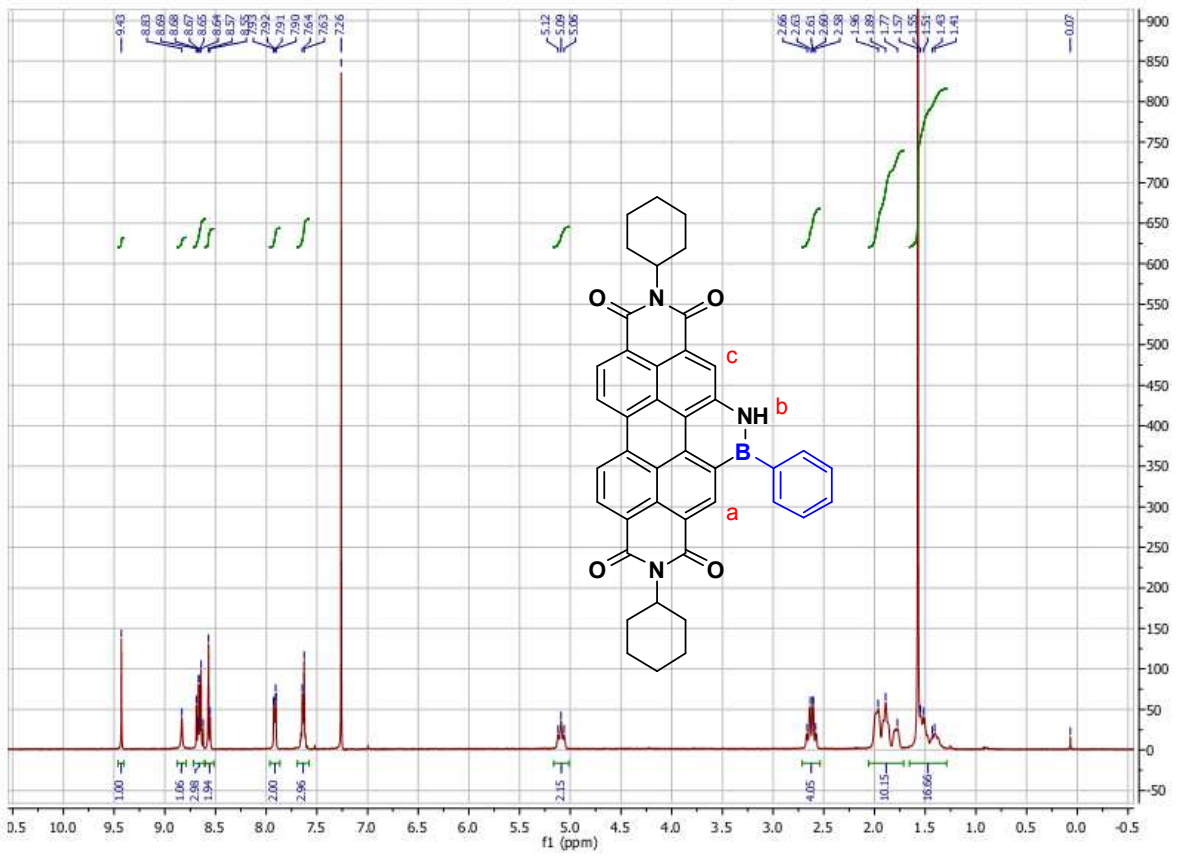


**Figure S1** $^{1}$H NMR of compound **PDI-1BN** in *d*-chloroform**.**

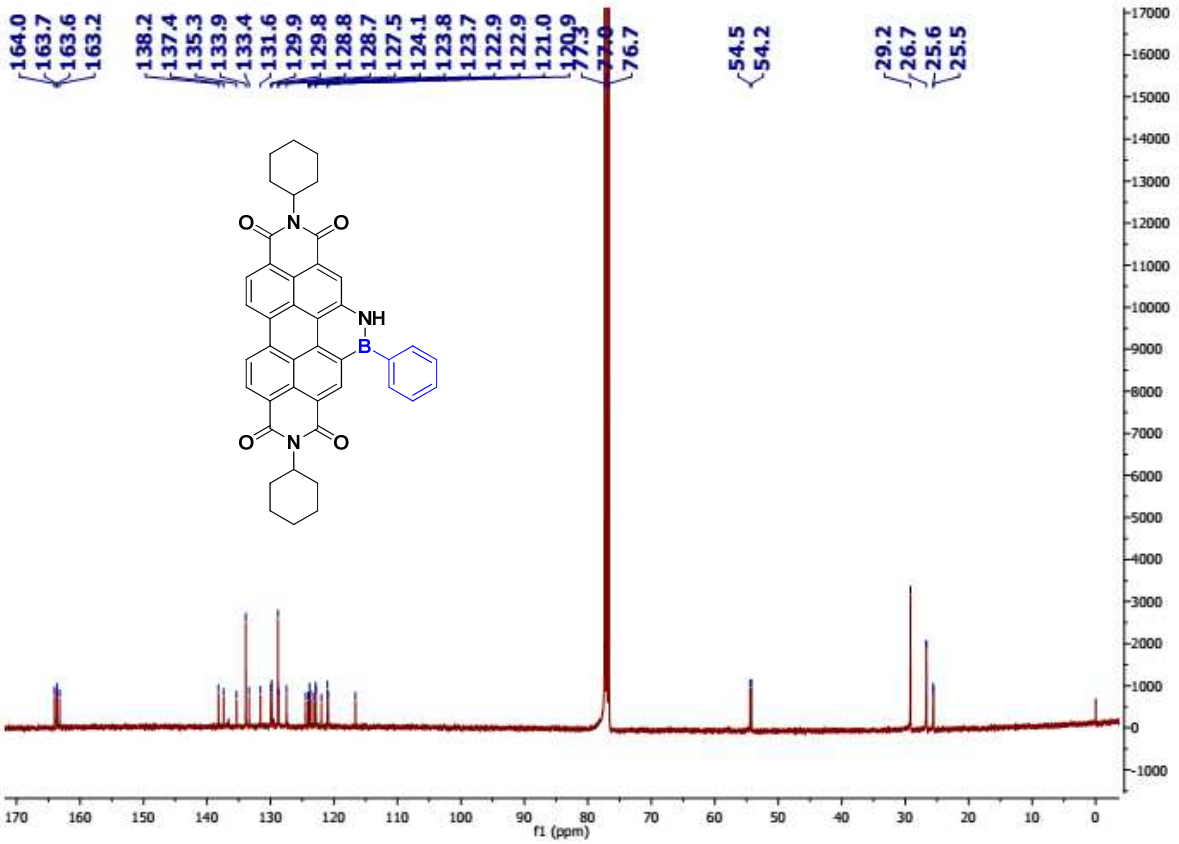


**Figure S2**[13]C NMR of compound **PDI-1BN** in *d*-chloroform.

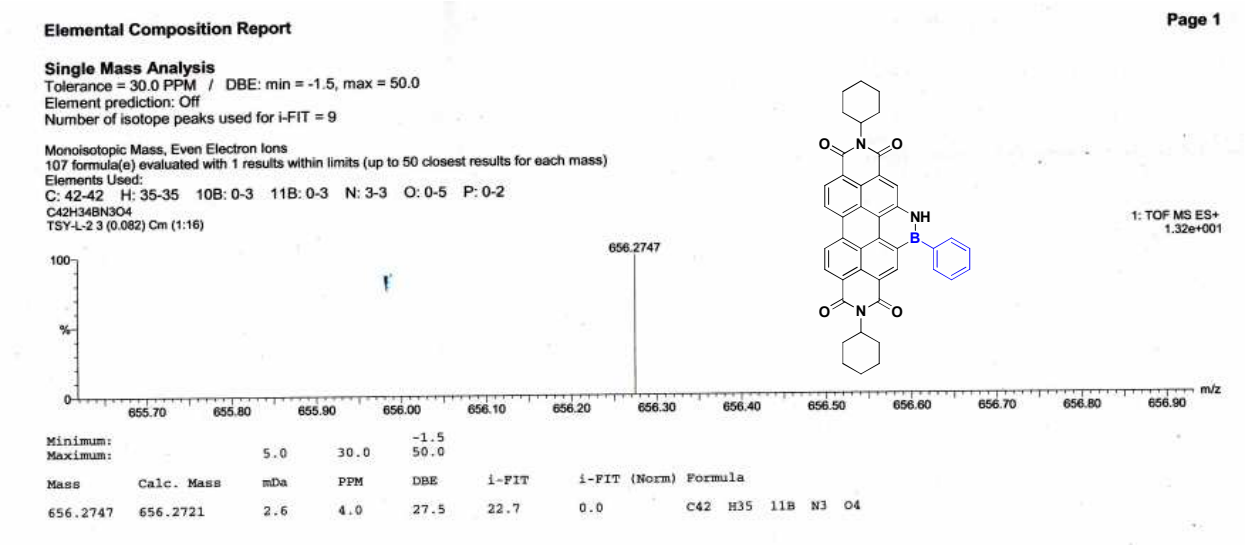


**Figure S3** HRMS of compound **PDI-1BN.**

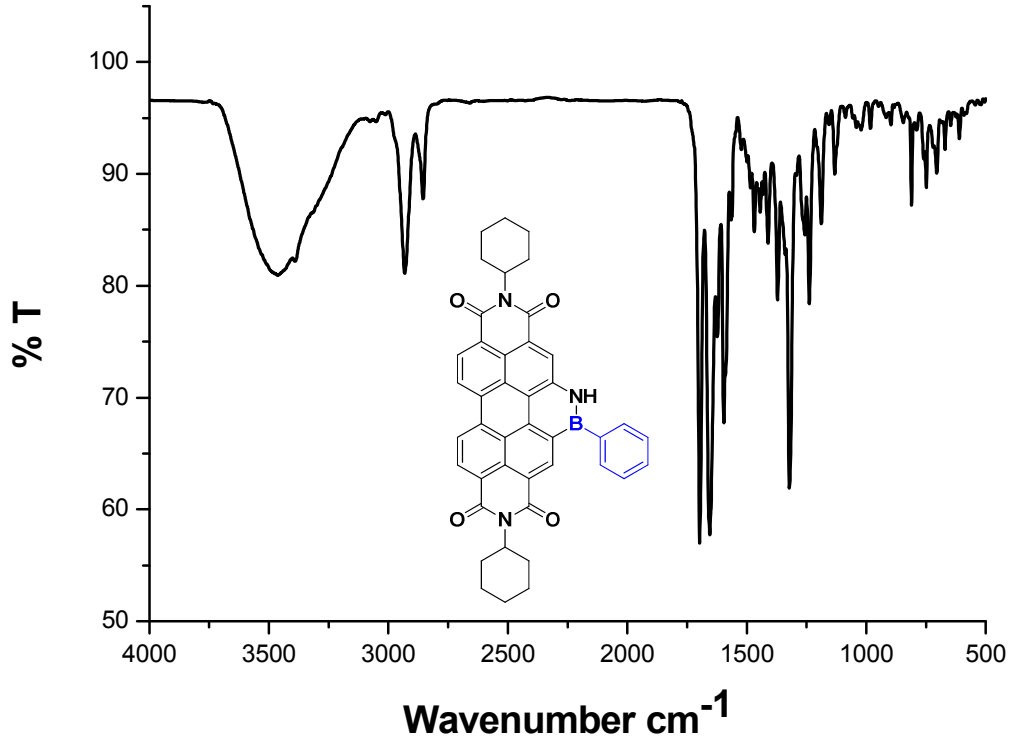


**Figure S4** Infrared spectrum of compound **PDI-1BN**.

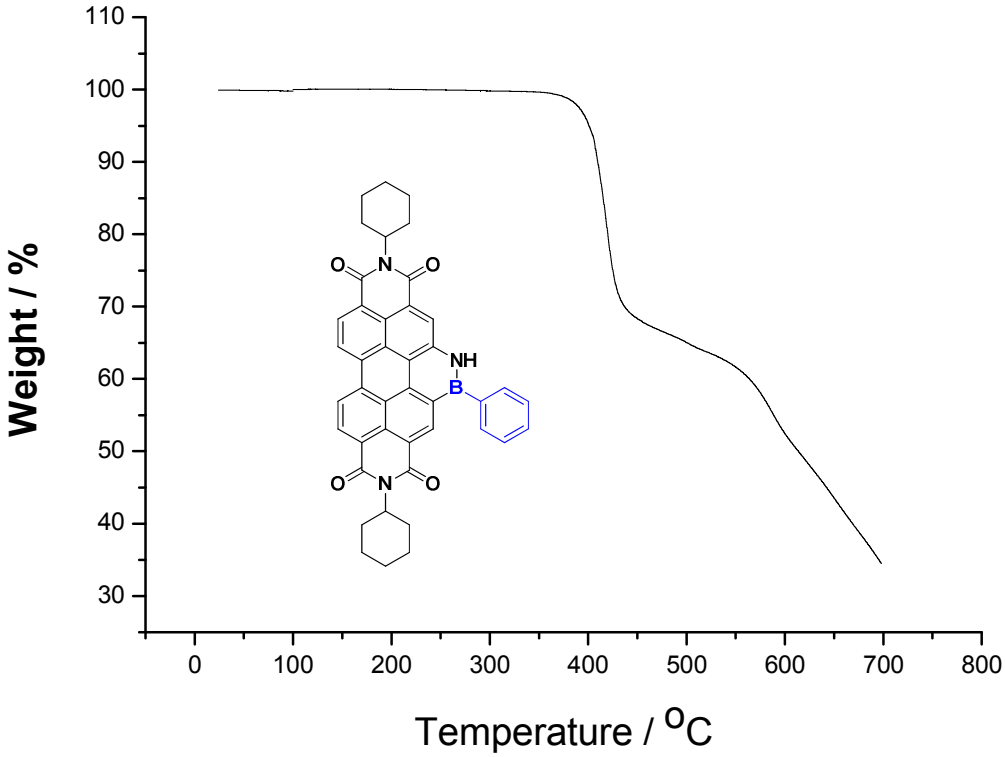


**Figure S5** Thermogravimetric analysis (TGA) curve of compound **PDI-1BN**.

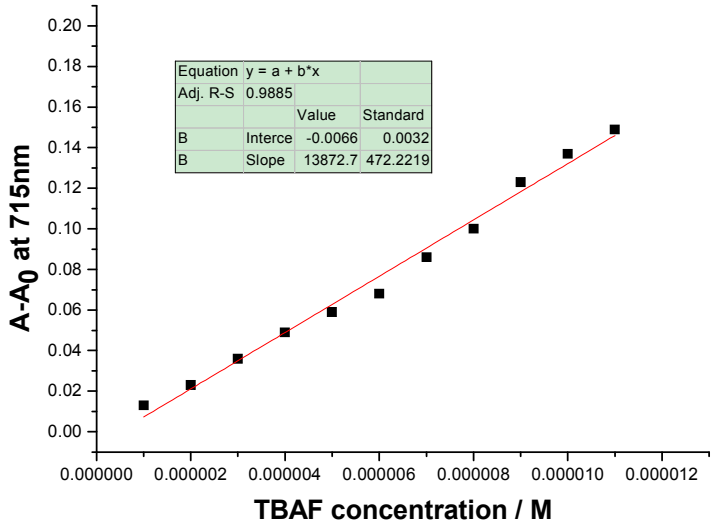


**Figure S6** The Absorption intensity increment at 715 nm of the probe ($1\times10^{-5}$ M) as a function of fluoride concentration in chloroform. Fluoride concentration: 1 - 11μM (the lower concentration part).

The method for determining the detection limit:

First the calibration curve was obtained from the plot of absorption intensity increment, A-A0, as a function of the analyte concentration (fluoride anion). The regression curve equation was then obtained for the lower concentration part.

The detection limit = 3 × S.D./ k

where k is the slope of the curve equation, and S.D. represents the standard deviation for the probe solution intensity increment in the absence of fluoride anion.

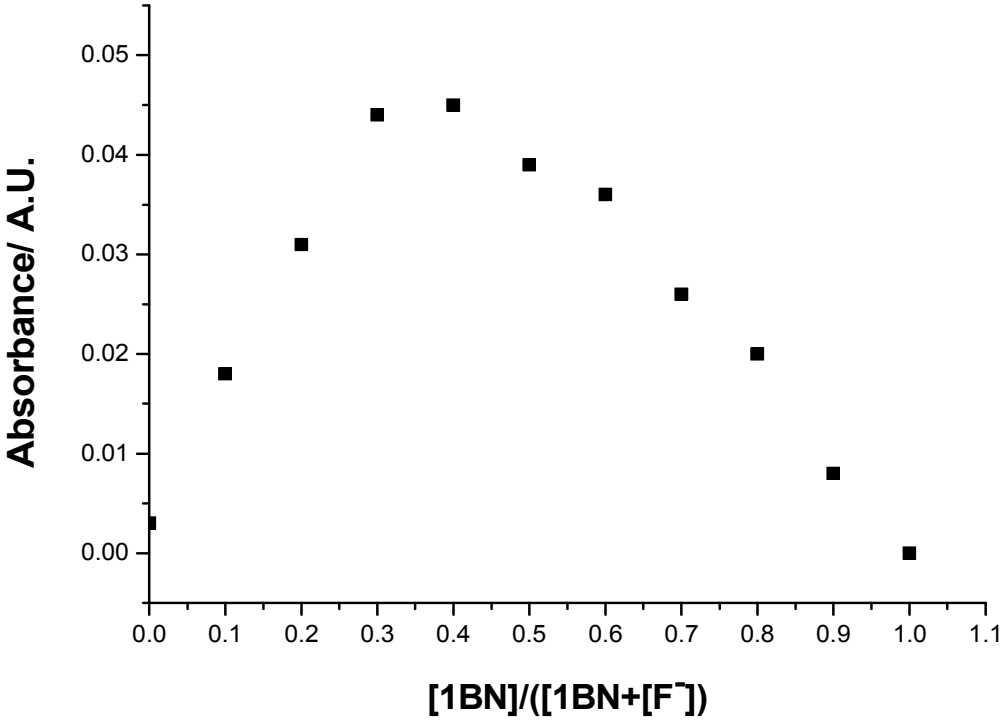


**Figure S7** Job's plots according to the method for continuous variations. The total concentration of **PDI-1BN** and fluoride is $2\times10^{-5}$M.

## Calculation

Electronic structure of 1BN can be theoretically investigated by quantum chemistry calculation using Gaussian09, The molecular geometries of 1BN in ground state was optimized by density functional theory according to the B3LYP/6-31G* and B3PW91//B3LYP/6-31G* level, The calculated results of HOMO, LUMO and bandgap are shown in the Table S1.

**Table S1.**The HOMO, LUMO and band gap of PDI-1BN at different theoretical level

| PDI-1BN | HOMO (eV) | LUMO (eV) | Bandgap (eV) |
|---|---|---|---|
| B3LYP/6-31G* | -5.84 | -3.24 | 2.60 |
| B3PW91//B3LYP/6-31G* | -5.97 | -3.36 | 2.61 |

**Table S2**. The absolute energies of HOMO and LUMO orbitals:

| PDI-1BN | HOMO (hatree) | LUMO (hatree) |
|---|---|---|
| B3LYP/6-31G* | -0.21482 | -0.11900 |
| B3PW91//B3LYP/6-31G* | -0.21963 | -0.12347 |

**Table S3**.The coordinates of 1BN in ground state optimized at B3LYP/6-31G* level:

| | X | Y | Z |
|---|---|---|---|
| C | 1.042770000 | -0.004980000 | 2.287439000 |
| C | 0.961555000 | -0.759337000 | 3.477355000 |
| C | 0.926619000 | -0.113563000 | 4.736252000 |
| C | 0.967979000 | 1.257572000 | 4.824343000 |
| C | 1.040720000 | 2.049900000 | 3.647588000 |
| C | 1.077349000 | 1.420305000 | 2.370314000 |
| C | 1.149423000 | 2.229100000 | 1.195270000 |
| C | 1.180856000 | 3.621550000 | 1.348584000 |
| C | 1.144473000 | 4.227668000 | 2.604873000 |
| C | 1.075768000 | 3.452624000 | 3.756352000 |
| H | 0.869774000 | -0.694049000 | 5.652621000 |
| H | 1.169770000 | 5.307320000 | 2.704100000 |
| H | 1.235883000 | 4.262589000 | 0.476435000 |
| C | 1.267686000 | 0.257642000 | -2.629883000 |
| C | 1.292214000 | 1.645090000 | -2.554355000 |
| C | 1.253021000 | 2.288958000 | -1.317942000 |
| C | 1.187409000 | 1.572233000 | -0.115623000 |
| C | 1.158096000 | 0.144476000 | -0.177144000 |
| C | 1.199444000 | -0.502692000 | -1.446219000 |
| C | 1.162661000 | -1.921115000 | -1.524491000 |
| C | 1.086993000 | -2.672658000 | -0.371538000 |
| C | 1.064443000 | -2.076783000 | 0.915361000 |
| C | 1.090627000 | -0.662295000 | 1.004623000 |
| H | 1.343632000 | 2.213110000 | -3.477027000 |
| H | 1.275101000 | 3.372416000 | -1.306482000 |

| | | | |
|---|---|---|---|
| H | 1.041670000 | -3.751601000 | -0.470226000 |
| N | 0.928004000 | -2.135232000 | 3.410664000 |
| H | 0.898927000 | -2.603880000 | 4.310577000 |
| B | 0.987655000 | -2.910837000 | 2.211362000 |
| C | 0.954062000 | -4.472140000 | 2.345012000 |
| C | 1.833648000 | -5.309352000 | 1.631144000 |
| C | 0.046968000 | -5.091728000 | 3.228110000 |
| C | 1.811124000 | -6.694992000 | 1.792172000 |
| C | 0.010757000 | -6.477081000 | 3.386031000 |
| C | 0.896267000 | -7.282810000 | 2.667679000 |
| H | 2.559655000 | -4.871236000 | 0.950824000 |
| H | -0.659693000 | -4.480575000 | 3.787434000 |
| H | 2.506328000 | -7.315831000 | 1.233228000 |
| H | -0.707995000 | -6.927769000 | 4.065665000 |
| H | 0.872595000 | -8.362660000 | 2.788713000 |
| C | 1.041641000 | 4.118952000 | 5.083323000 |
| O | 1.061817000 | 5.339574000 | 5.180703000 |
| C | 0.938979000 | 1.891484000 | 6.168943000 |
| O | 0.876903000 | 1.212452000 | 7.186317000 |
| N | 0.989185000 | 3.296735000 | 6.221895000 |
| C | 0.974052000 | 3.920338000 | 7.579116000 |
| C | -0.296688000 | 4.748950000 | 7.835552000 |
| C | -0.305392000 | 5.263454000 | 9.285299000 |
| C | 0.968174000 | 6.059039000 | 9.610154000 |
| C | 2.229719000 | 5.228289000 | 9.329827000 |
| C | 2.257432000 | 4.714018000 | 7.880291000 |
| H | 0.949817000 | 3.059599000 | 8.249841000 |
| H | -1.181301000 | 4.127074000 | 7.648310000 |
| H | -0.334615000 | 5.593988000 | 7.141409000 |
| H | -1.195720000 | 5.882874000 | 9.450388000 |
| H | -0.385457000 | 4.410699000 | 9.975671000 |
| H | 0.954307000 | 6.385270000 | 10.657812000 |
| H | 0.991431000 | 6.970831000 | 8.995842000 |
| H | 3.130458000 | 5.823255000 | 9.525641000 |
| H | 2.262835000 | 4.374342000 | 10.022639000 |
| H | 3.131126000 | 4.068757000 | 7.722901000 |
| H | 2.342026000 | 5.558092000 | 7.189644000 |
| C | 1.317536000 | -0.397575000 | -3.961035000 |
| O | 1.374058000 | 0.265693000 | -4.990511000 |
| C | 1.212899000 | -2.608887000 | -2.838835000 |
| O | 1.187299000 | -3.830236000 | -2.922173000 |
| N | 1.303894000 | -1.799388000 | -3.992146000 |
| C | 1.399796000 | -2.505035000 | -5.304169000 |
| C | 2.732838000 | -2.227820000 | -6.021108000 |
| C | 2.826697000 | -3.067206000 | -7.306516000 |
| C | 1.622557000 | -2.821700000 | -8.228778000 |

| | | | |
|---|---|---|---|
| C | 0.298126000 | -3.084646000 | -7.496218000 |
| C | 0.184589000 | -2.245041000 | -6.211885000 |
| H | 1.384963000 | -3.559788000 | -5.024218000 |
| H | 3.565277000 | -2.469647000 | -5.348007000 |
| H | 2.806307000 | -1.164684000 | -6.267938000 |
| H | 3.762750000 | -2.835778000 | -7.830116000 |
| H | 2.870366000 | -4.135060000 | -7.045539000 |
| H | 1.693725000 | -3.455737000 | -9.121758000 |
| H | 1.641513000 | -1.779628000 | -8.579494000 |
| H | -0.552458000 | -2.867382000 | -8.154297000 |
| H | 0.231710000 | -4.152807000 | -7.241641000 |
| H | -0.735139000 | -2.500841000 | -5.670583000 |
| H | 0.133589000 | -1.181989000 | -6.465498000 |