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Coordination of the ambiphilic phosphinoborane $t\text{Bu}_2\text{PCH}_2\text{BPh}_2$ to $\text{Cu}(\text{I})\text{Cl}$

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Supporting Information

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|-----------|------------------------------|-----------|
| 1. | NMR spectra | S2 |
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1. NMR spectra

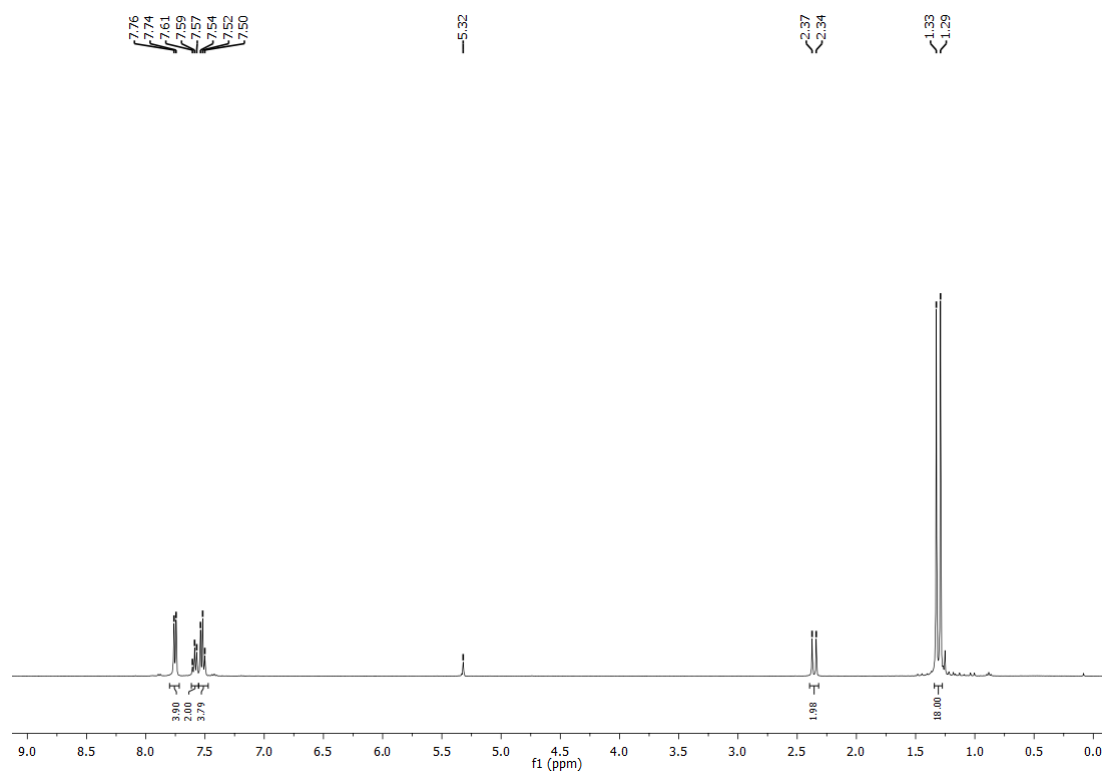


Figure S1: ^1H NMR spectrum of compound **2**

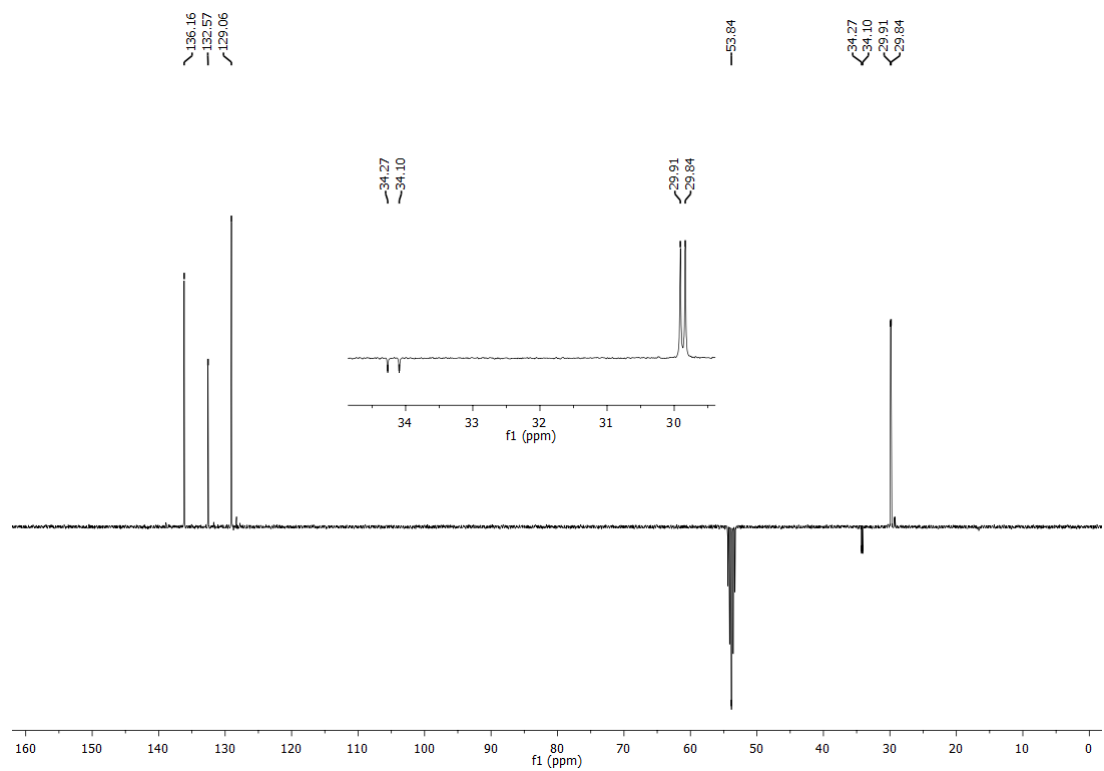


Figure S2: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **2**

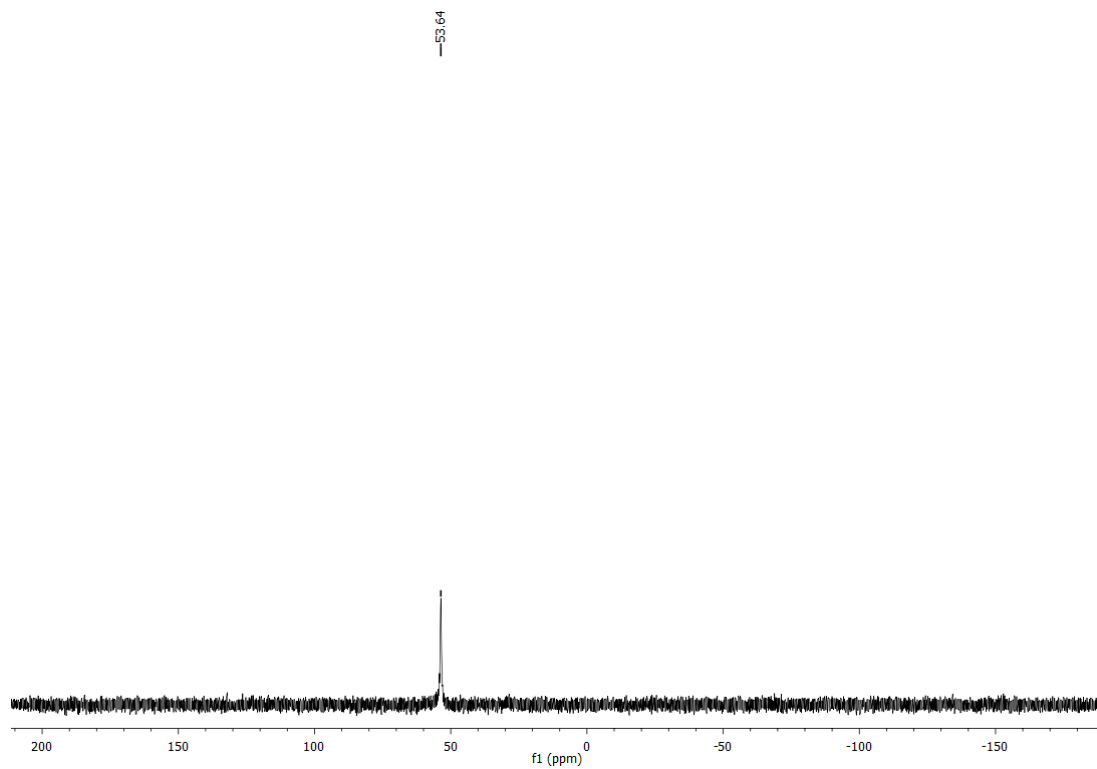


Figure S3: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **2**

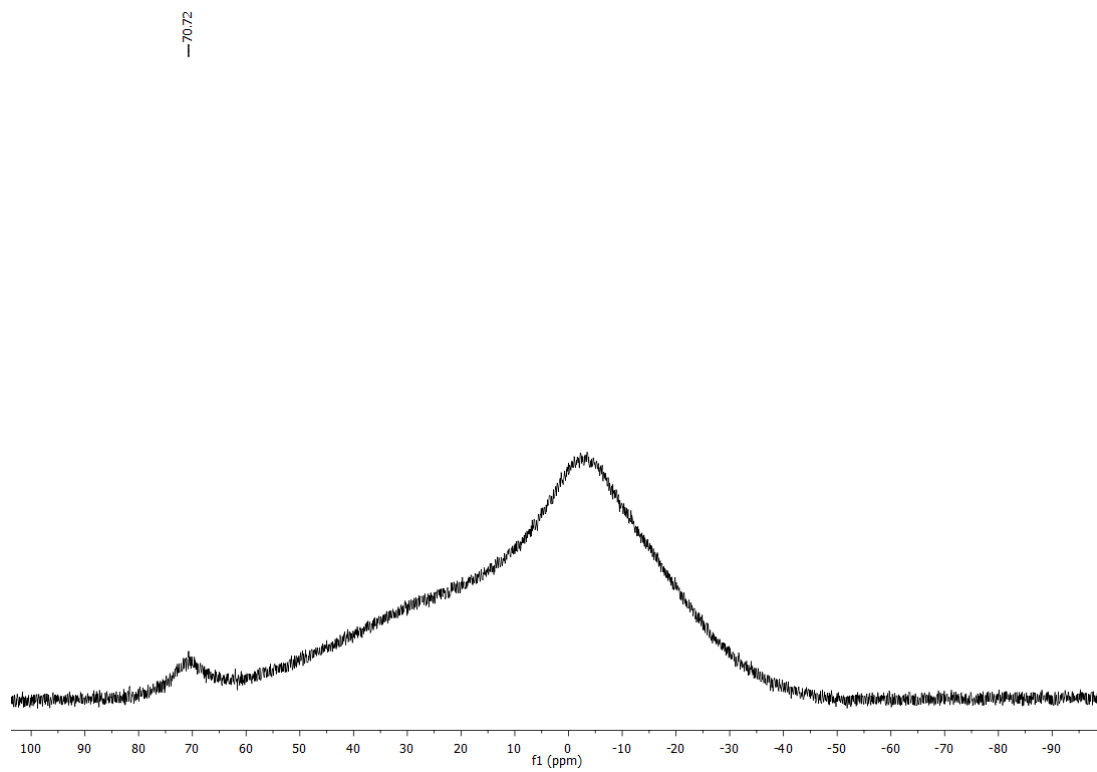


Figure S4: $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **2**

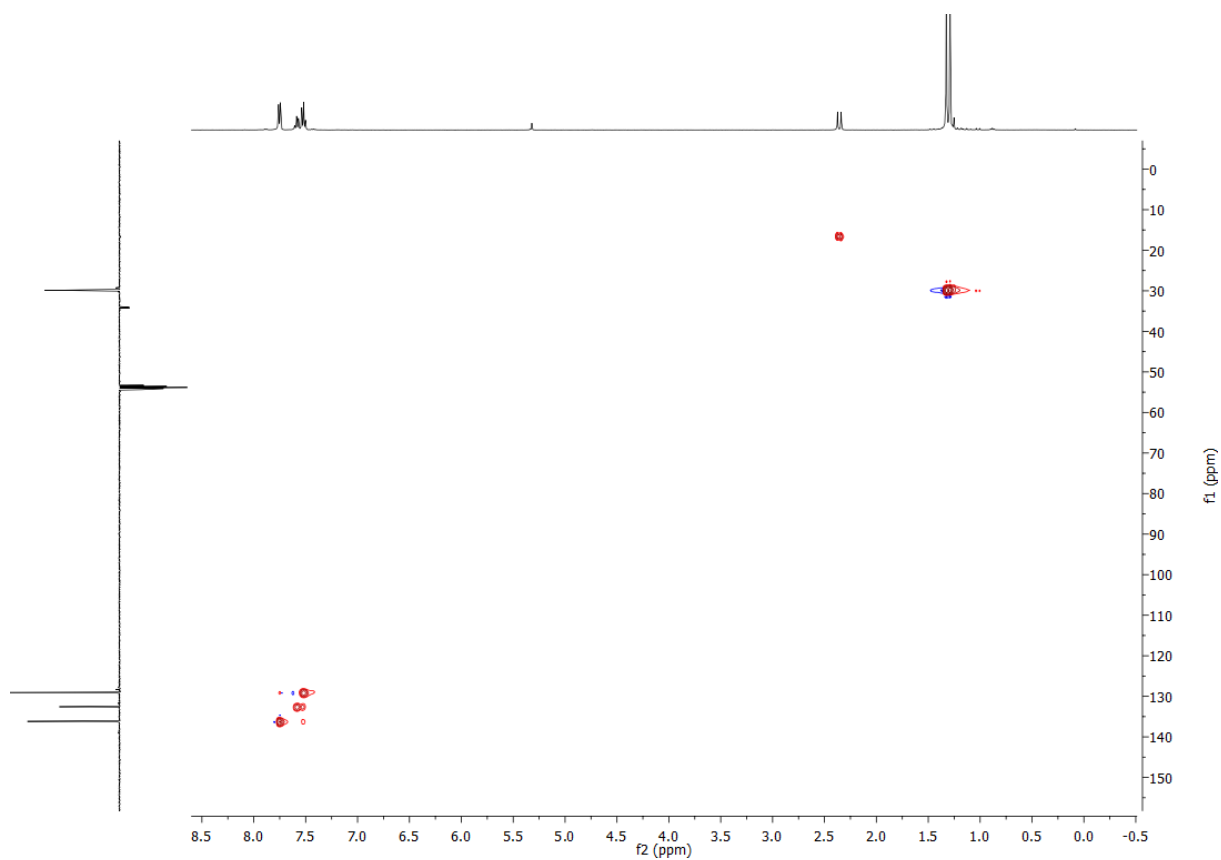


Figure S5: HSQC NMR spectrum of compound **2**

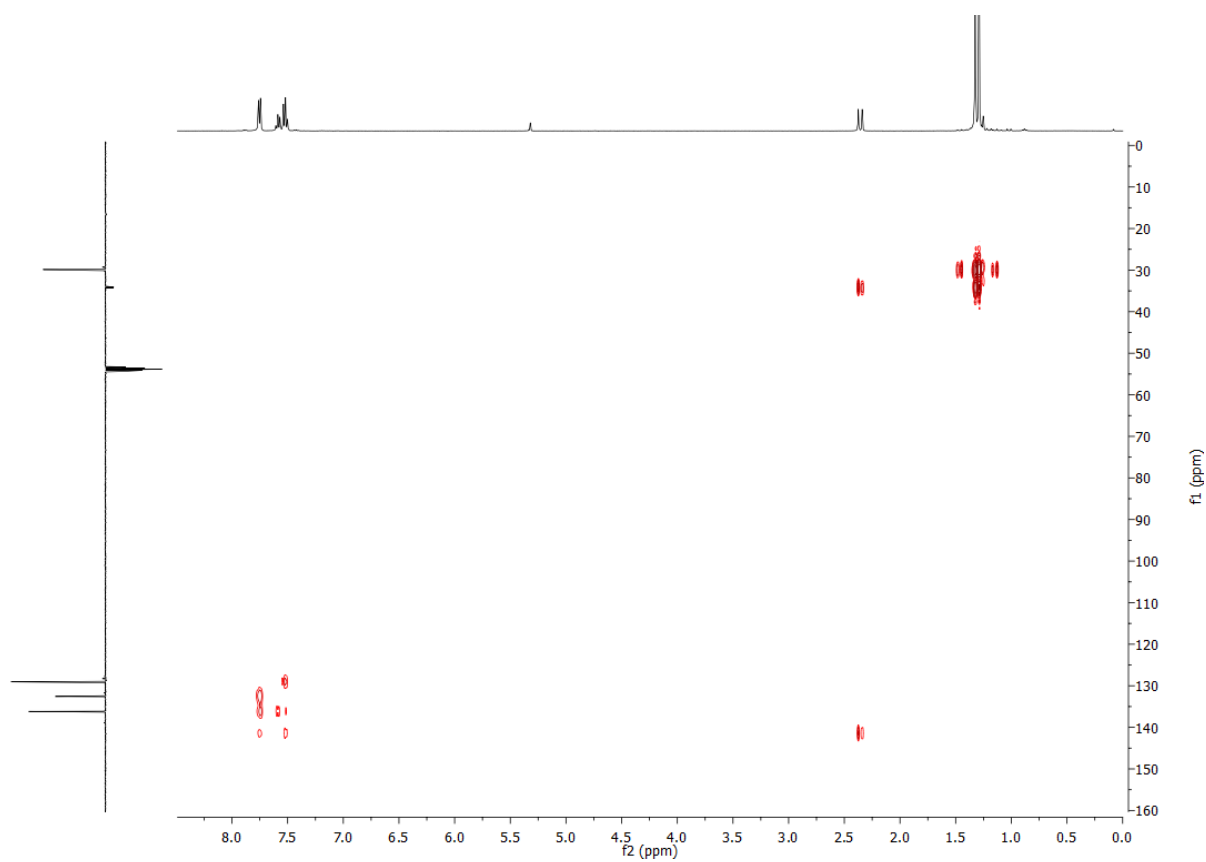


Figure S6: HMBC NMR spectrum of compound **2**

2. Computational details

Optimized geometry (Cartesian coordinates) and uncorrected energy (in a.u.) for **2**.

E = -6570.38609488

| | | | |
|----|--------------|--------------|--------------|
| Cl | -0.563717000 | 0.656848000 | -1.645954000 |
| Cu | -1.274516000 | -0.598037000 | 0.227346000 |
| P | -3.170264000 | -1.790881000 | 0.240864000 |
| B | -4.806039000 | 0.634458000 | 0.605813000 |
| C | -4.636665000 | -0.906681000 | 0.947696000 |
| H | -5.548369000 | -1.489763000 | 0.782598000 |
| H | -4.466159000 | -0.922742000 | 2.035933000 |
| C | -3.089725000 | -3.345227000 | 1.318698000 |
| C | -4.443431000 | -4.013349000 | 1.600759000 |
| H | -4.931610000 | -4.381605000 | 0.695888000 |
| H | -5.134868000 | -3.335224000 | 2.110913000 |
| H | -4.285269000 | -4.873995000 | 2.263159000 |
| C | -2.480414000 | -2.890807000 | 2.660313000 |
| H | -3.108890000 | -2.154558000 | 3.175006000 |
| H | -1.485060000 | -2.454976000 | 2.529585000 |
| H | -2.392980000 | -3.759079000 | 3.325840000 |
| C | -2.127973000 | -4.362282000 | 0.688458000 |
| H | -2.549825000 | -4.825800000 | -0.209081000 |
| H | -1.925169000 | -5.165045000 | 1.408511000 |
| H | -1.170738000 | -3.894742000 | 0.431675000 |
| C | -3.682322000 | -2.182963000 | -1.534646000 |
| C | -4.089010000 | -0.837903000 | -2.166079000 |
| H | -3.323449000 | -0.068978000 | -2.011289000 |
| H | -5.045319000 | -0.470099000 | -1.782225000 |
| H | -4.207921000 | -0.973068000 | -3.248266000 |
| C | -2.452141000 | -2.696859000 | -2.305328000 |
| H | -1.645367000 | -1.956850000 | -2.290283000 |
| H | -2.731136000 | -2.870808000 | -3.352548000 |
| H | -2.066163000 | -3.638562000 | -1.905917000 |
| C | -4.837799000 | -3.179918000 | -1.675324000 |
| H | -5.705330000 | -2.900569000 | -1.066275000 |
| H | -4.536391000 | -4.195222000 | -1.399076000 |
| H | -5.166549000 | -3.210395000 | -2.721994000 |
| C | -3.584816000 | 1.601245000 | 0.774690000 |
| C | -3.380363000 | 2.670125000 | -0.114026000 |
| H | -4.086535000 | 2.830086000 | -0.924685000 |

| | | | |
|----|--------------|--------------|--------------|
| C | -2.281262000 | 3.514219000 | 0.003906000 |
| H | -2.135589000 | 4.317211000 | -0.712513000 |
| C | -1.367201000 | 3.323963000 | 1.036053000 |
| H | -0.514472000 | 3.988812000 | 1.141719000 |
| C | -1.542362000 | 2.274291000 | 1.933475000 |
| H | -0.819869000 | 2.100576000 | 2.724447000 |
| C | -2.629200000 | 1.416387000 | 1.791585000 |
| H | -2.738379000 | 0.599450000 | 2.501846000 |
| C | -6.217340000 | 1.197651000 | 0.211484000 |
| C | -6.545694000 | 2.544195000 | 0.451016000 |
| H | -5.802812000 | 3.199967000 | 0.895765000 |
| C | -7.803083000 | 3.055372000 | 0.144930000 |
| H | -8.029042000 | 4.098026000 | 0.348626000 |
| C | -8.766755000 | 2.230344000 | -0.428117000 |
| H | -9.746892000 | 2.628233000 | -0.675655000 |
| C | -8.472370000 | 0.891516000 | -0.678558000 |
| H | -9.221065000 | 0.242676000 | -1.123772000 |
| C | -7.220487000 | 0.386306000 | -0.348894000 |
| H | -7.016779000 | -0.663245000 | -0.547373000 |
| Cl | 0.564177000 | -0.666697000 | 1.644515000 |
| Cu | 1.274546000 | 0.588733000 | -0.227435000 |
| P | 3.165413000 | 1.789329000 | -0.247418000 |
| B | 4.810122000 | -0.631833000 | -0.600202000 |
| C | 4.635921000 | 0.907332000 | -0.948408000 |
| H | 5.545339000 | 1.494370000 | -0.784801000 |
| H | 4.466825000 | 0.917932000 | -2.036932000 |
| C | 3.079081000 | 3.337255000 | -1.333893000 |
| C | 4.429914000 | 4.010691000 | -1.617196000 |
| H | 4.913354000 | 4.388792000 | -0.713842000 |
| H | 5.126664000 | 3.332464000 | -2.119939000 |
| H | 4.268963000 | 4.865185000 | -2.286849000 |
| C | 2.474815000 | 2.872354000 | -2.674246000 |
| H | 3.108431000 | 2.137036000 | -3.183969000 |
| H | 1.481617000 | 2.431811000 | -2.543115000 |
| H | 2.383799000 | 3.736611000 | -3.344490000 |
| C | 2.110929000 | 4.352782000 | -0.711006000 |
| H | 2.528560000 | 4.822791000 | 0.185161000 |
| H | 1.906068000 | 5.151060000 | -1.435456000 |
| H | 1.155286000 | 3.882019000 | -0.454118000 |
| C | 3.674541000 | 2.193148000 | 1.526298000 |
| C | 4.086392000 | 0.853202000 | 2.165203000 |
| H | 3.323650000 | 0.080592000 | 2.014697000 |
| H | 5.043968000 | 0.486754000 | 1.783235000 |
| H | 4.204929000 | 0.994709000 | 3.246624000 |

| | | | |
|---|-------------|--------------|--------------|
| C | 2.441346000 | 2.705539000 | 2.293045000 |
| H | 1.637708000 | 1.962127000 | 2.280091000 |
| H | 2.718035000 | 2.885412000 | 3.339872000 |
| H | 2.051960000 | 3.643709000 | 1.888654000 |
| C | 4.825258000 | 3.196144000 | 1.662756000 |
| H | 5.694893000 | 2.917337000 | 1.056451000 |
| H | 4.519258000 | 4.208304000 | 1.380048000 |
| H | 5.152407000 | 3.234391000 | 2.709663000 |
| C | 3.592187000 | -1.603269000 | -0.766127000 |
| C | 3.391799000 | -2.670417000 | 0.125596000 |
| H | 4.098828000 | -2.825683000 | 0.936423000 |
| C | 2.295707000 | -3.518764000 | 0.010289000 |
| H | 2.153248000 | -4.320460000 | 0.728790000 |
| C | 1.380565000 | -3.334462000 | -1.021945000 |
| H | 0.530582000 | -4.003085000 | -1.125664000 |
| C | 1.551441000 | -2.286451000 | -1.922166000 |
| H | 0.827914000 | -2.117653000 | -2.713292000 |
| C | 2.635432000 | -1.424424000 | -1.783107000 |
| H | 2.741600000 | -0.609229000 | -2.495826000 |
| C | 6.223017000 | -1.188726000 | -0.202583000 |
| C | 6.556342000 | -2.534916000 | -0.437312000 |
| H | 5.816100000 | -3.194763000 | -0.880470000 |
| C | 7.815237000 | -3.040628000 | -0.128306000 |
| H | 8.045063000 | -4.083138000 | -0.328376000 |
| C | 8.775415000 | -2.210247000 | 0.442861000 |
| H | 9.756727000 | -2.603806000 | 0.692691000 |
| C | 8.476073000 | -0.871641000 | 0.688570000 |
| H | 9.222078000 | -0.218661000 | 1.132249000 |
| C | 7.222754000 | -0.371927000 | 0.355987000 |
| H | 7.015278000 | 0.677567000 | 0.550810000 |