

## **Supporting Information**

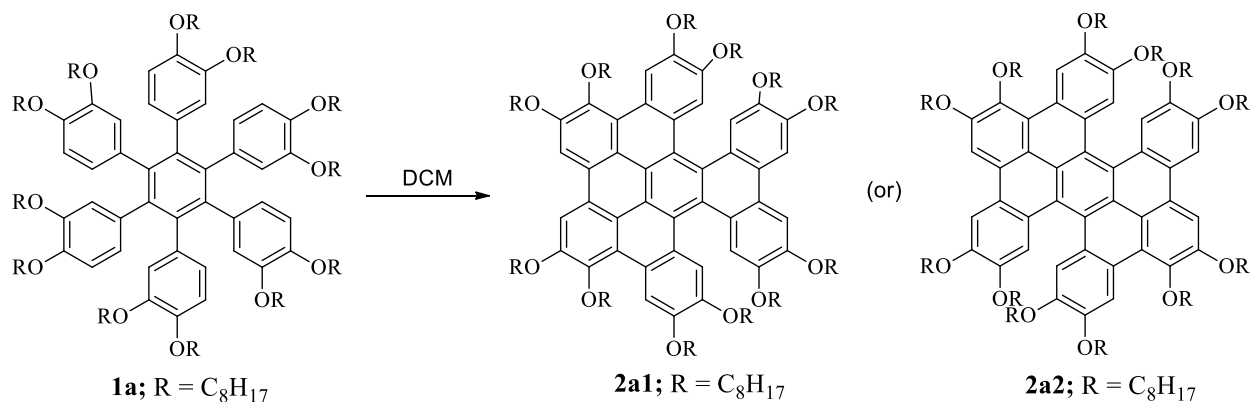
### **Scholl Reaction of Hexaphenylbenzenes with Hexakis-alkoxy Substituents**

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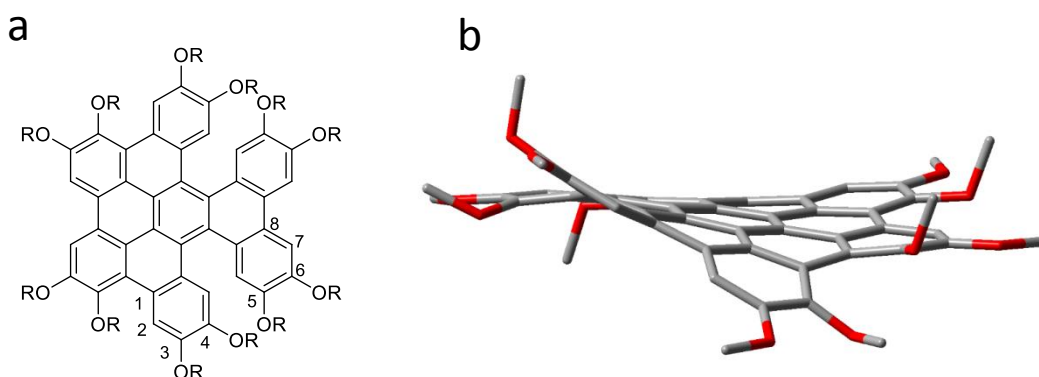
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**Table S1.** Scholl reaction and product obtained under various conditions.

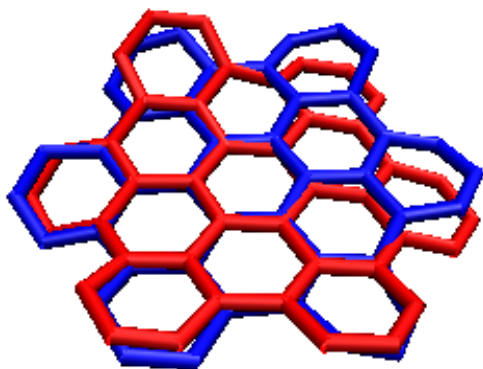


| Entry | Reagent                                                       | Temperature (°C) | Time (h) <sup>a</sup> |
|-------|---------------------------------------------------------------|------------------|-----------------------|
| 1     | DDQ (6 equiv.)/CH <sub>3</sub> COOH                           | 0                | 2                     |
| 2     | DDQ (6 equiv.)/CF <sub>3</sub> COOH                           | 0                | 2                     |
| 3     | DDQ (6 equiv.)/CF <sub>3</sub> SO <sub>3</sub> H              | 0                | 2                     |
| 4     | DDQ (6 equiv.)/CH <sub>3</sub> COOH                           | 0                | 24 <sup>b</sup>       |
| 5     | DDQ (6 equiv.)/CH <sub>3</sub> COOH                           | 22               | 2                     |
| 6     | DDQ (12 equiv.)/CH <sub>3</sub> COOH                          | 0                | 2                     |
| 7     | FeCl <sub>3</sub> (12 equiv.)/CH <sub>3</sub> NO <sub>2</sub> | 22               | 2                     |
| 8     | FeCl <sub>3</sub> (20 equiv.)/CH <sub>3</sub> NO <sub>2</sub> | 22               | 2                     |
| 9     | VOCl <sub>3</sub> (5 equiv.)                                  | 22               | 2                     |
| 10    | DDQ (6 equiv.)/CH <sub>3</sub> COOH                           | Reflux           | 2                     |

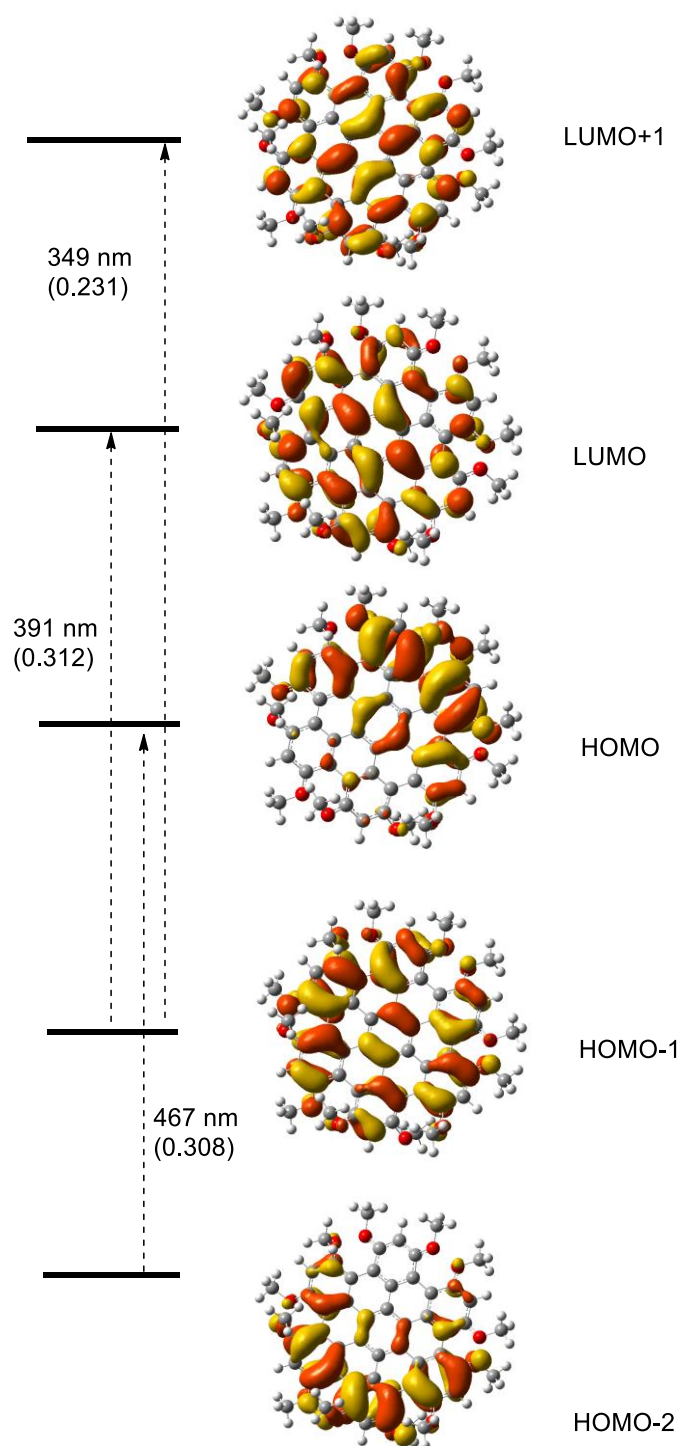
<sup>a</sup>TLC monitoring till completion of reactant. <sup>b</sup>Extended reaction time after completion of reactant.



**Figure S1** (a) The schematic diagram of **2c1** to show the puckered portion of the ring is analogous to the 4,5 position of phenanthrene. Not surprisingly, **2c2** also exhibits similar puckering. (b) to exhibit significant distortion involved in hypothetical fully-fused HBC core from o-bis-methoxy substituted substrates.



**Figure S2** Side view of the overlapped structures for computationally optimized **2d** (blue) and **3** (red). This image displays **2d** as a near planar ring where as **3** is significantly puckered. The methoxy substituents are omitted for clarity.



**Figure S3** The TD-DFT predicted dominant optical transitions for the partially fused molecule **2c1**. The oscillator strengths are reported in the parentheses for the respective transition.

## Cartesian Coordinates for Computationally Optimized Structures:

2c1

0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.70885000 | 1.37478200  | 0.16384300  |
| C | -1.40720900 | 0.16717300  | 0.00443500  |
| C | -0.68722700 | -1.06235300 | 0.05001000  |
| C | 0.70099700  | -1.05505700 | 0.29582600  |
| C | 1.42297100  | 0.15202900  | -0.03123100 |
| C | 0.70423500  | 1.36541000  | -0.13287300 |
| C | -1.44654400 | 2.51384700  | 0.70289900  |
| C | -2.87734600 | 2.51550400  | 0.69182100  |
| C | -3.53301100 | 3.62858400  | 1.29777400  |
| C | -2.81133000 | 4.67186300  | 1.88185200  |
| C | -1.41640200 | 4.60912900  | 1.95333400  |
| C | -0.75586500 | 3.54027100  | 1.38646600  |
| C | -2.84479200 | 0.15275200  | -0.09102000 |
| C | -3.51603000 | -1.06331900 | -0.44331700 |
| C | -4.92334500 | -1.10832100 | -0.37711900 |
| C | -5.64229000 | 0.10419900  | -0.23982300 |
| C | -4.97951600 | 1.29897500  | -0.01385400 |
| C | -3.58159000 | 1.34147200  | 0.16264600  |
| H | -5.54347300 | 2.20738200  | 0.11121700  |
| C | -1.37480400 | -2.30285800 | -0.19557300 |
| C | -0.66089000 | -3.52190800 | -0.12647500 |
| C | -1.20931100 | -4.67165500 | -0.71552900 |
| C | -2.39898600 | -4.58337800 | -1.42865400 |
| C | -3.13398000 | -3.37255200 | -1.45920000 |
| C | -2.70790100 | -2.26692500 | -0.70416100 |
| H | -0.66263500 | -5.60509600 | -0.67896100 |
| C | 1.25575200  | -2.28659500 | 0.85815000  |
| C | 2.37926300  | -2.28847000 | 1.71382900  |
| C | 2.88980200  | -3.45615600 | 2.25091500  |
| C | 2.25312100  | -4.68966400 | 1.97111500  |
| C | 1.12675000  | -4.70381900 | 1.16777000  |
| C | 0.59582400  | -3.52176800 | 0.61158700  |
| H | 0.62908000  | -5.65709500 | 1.02443500  |
| C | 2.85989800  | 0.17491500  | -0.32331500 |
| C | 3.57284200  | 1.40724900  | -0.37834000 |
| C | 4.99063700  | 1.36313700  | -0.34921000 |
| C | 5.69022900  | 0.17065400  | -0.43604900 |
| C | 4.97135700  | -1.03128200 | -0.64693500 |
| C | 3.59450600  | -1.00574900 | -0.58322900 |
| H | 5.52492500  | 2.29412700  | -0.26474500 |
| C | 1.39022800  | 2.55829200  | -0.63700600 |
| C | 0.65026600  | 3.60815300  | -1.22426300 |
| C | 1.24769800  | 4.78364500  | -1.62952400 |
| C | 2.62874200  | 4.93791400  | -1.48517200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.41012800  | 3.87111800  | -1.03297400 |
| C | 2.81733600  | 2.64015000  | -0.62172400 |
| O | -7.00714600 | -0.00316400 | -0.28256100 |
| C | -7.78270700 | 1.17487400  | -0.14453400 |
| H | -7.62705500 | 1.64921800  | 0.83321400  |
| H | -7.55866000 | 1.90325900  | -0.93469300 |
| H | -8.82373400 | 0.85676700  | -0.23013900 |
| O | -5.53746600 | -2.31563000 | -0.29740600 |
| C | -6.70086300 | -2.61900800 | -1.07490800 |
| H | -6.67840400 | -2.10935900 | -2.04185700 |
| H | -6.67037200 | -3.69742300 | -1.23986100 |
| H | -7.60907600 | -2.34028000 | -0.53546800 |
| O | -3.45554400 | 5.72896000  | 2.48951000  |
| C | -4.09166900 | 6.64539300  | 1.59397300  |
| H | -3.35738900 | 7.09660800  | 0.91359100  |
| H | -4.87712200 | 6.15305800  | 1.01209800  |
| H | -4.53003600 | 7.42632800  | 2.22015300  |
| O | 3.20685900  | 6.12086900  | -1.89652800 |
| C | 3.73555800  | 6.93072700  | -0.84178300 |
| H | 2.94334300  | 7.21528800  | -0.13698400 |
| H | 4.53567100  | 6.41214100  | -0.30417100 |
| H | 4.13315600  | 7.82941700  | -1.31959400 |
| O | 7.05044700  | 0.05827200  | -0.36377000 |
| C | 7.80239600  | 1.22938900  | -0.08631000 |
| H | 7.71305600  | 1.96893200  | -0.89305600 |
| H | 7.48928700  | 1.69136900  | 0.85842000  |
| H | 8.84172400  | 0.90484300  | -0.00722000 |
| O | 5.60131000  | -2.24384800 | -0.80356000 |
| C | 6.41505300  | -2.38814000 | -1.97011000 |
| H | 5.82093200  | -2.22626100 | -2.87925400 |
| H | 7.26309900  | -1.69723900 | -1.95654300 |
| H | 6.77938400  | -3.41800700 | -1.95698600 |
| O | 3.98199400  | -3.39105900 | 3.08781200  |
| C | 5.19385300  | -3.90725700 | 2.51480000  |
| H | 5.44493800  | -3.37450800 | 1.59013000  |
| H | 5.97377700  | -3.73895500 | 3.26141200  |
| H | 5.10561300  | -4.97954600 | 2.30833500  |
| O | 2.73194700  | -5.87988000 | 2.47234400  |
| C | 2.60481700  | -6.03208000 | 3.89116500  |
| H | 3.15184300  | -5.25002900 | 4.42636300  |
| H | 1.54798700  | -6.00974200 | 4.18803400  |
| H | 3.02699800  | -7.01126000 | 4.12947800  |
| O | -2.94761200 | -5.61176700 | -2.14279400 |
| C | -2.27625000 | -6.86109900 | -2.13825700 |
| H | -1.26966300 | -6.78264400 | -2.57036300 |
| H | -2.20077400 | -7.27387600 | -1.12375600 |
| H | -2.88351500 | -7.52748800 | -2.75374500 |
| O | -4.24267000 | -3.30460800 | -2.26824400 |
| C | -3.94110100 | -3.22846500 | -3.66384800 |
| H | -3.43394000 | -4.13274700 | -4.01558400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.90253100 | -3.13071900 | -4.17444800 |
| H | -3.32263100 | -2.34821200 | -3.88226800 |
| H | 0.32078500  | 3.47928100  | 1.47560200  |
| H | -0.41789000 | 3.49364900  | -1.35024100 |
| H | 2.87661200  | -1.36017100 | 1.96722500  |
| H | 3.08668900  | -1.94970100 | -0.71695100 |
| H | 0.67230000  | 5.59557800  | -2.06310600 |
| O | 4.78175400  | 4.05969100  | -1.01427500 |
| H | -0.88300800 | 5.39729200  | 2.47550400  |
| O | -4.91413600 | 3.72263300  | 1.35262100  |
| C | -5.46499000 | 3.40986200  | 2.64026900  |
| H | -5.06518800 | 4.08077100  | 3.40614900  |
| H | -6.54494700 | 3.55575300  | 2.55315700  |
| H | -5.25715800 | 2.36694900  | 2.90799400  |
| C | 5.39392600  | 4.06947300  | -2.31325300 |
| H | 6.45802700  | 4.25539700  | -2.14494300 |
| H | 5.26648900  | 3.09914800  | -2.80779600 |
| H | 4.97529500  | 4.86572300  | -2.93440100 |

## 2c2

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|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.39815000  | 0.39931000  | 0.10249600  |
| C | 0.40455500  | 1.41673800  | 0.14179400  |
| C | -0.97964300 | 1.08109200  | 0.18017300  |
| C | -1.36620400 | -0.26151300 | -0.06426400 |
| C | -0.37698700 | -1.27928700 | -0.09625100 |
| C | 1.00930300  | -0.94682000 | -0.12943500 |
| C | 2.76519000  | 0.82319200  | 0.44736800  |
| C | 3.17231300  | 2.16690700  | 0.23736300  |
| C | 4.48793000  | 2.54046600  | 0.59316000  |
| C | 5.36654200  | 1.64772600  | 1.18132500  |
| C | 4.92960700  | 0.33962100  | 1.47991300  |
| C | 3.65029600  | -0.04476600 | 1.12173300  |
| H | 4.82538800  | 3.55459700  | 0.43619900  |
| C | 0.79795300  | 2.80710500  | 0.00588100  |
| C | -0.19606000 | 3.81381900  | -0.08120200 |
| C | 0.15164500  | 5.09538400  | -0.53363600 |
| C | 1.46616100  | 5.39333200  | -0.87093800 |
| C | 2.48154800  | 4.43225000  | -0.67765800 |
| C | 2.17126500  | 3.15148400  | -0.19176400 |
| C | -1.90711200 | 2.14674500  | 0.58324200  |
| C | -3.11338700 | 1.86551500  | 1.26561000  |
| C | -3.98375500 | 2.86915700  | 1.65887800  |
| C | -3.66069100 | 4.22100400  | 1.36742000  |
| C | -2.45186000 | 4.50755600  | 0.76494700  |
| C | -1.53952800 | 3.49747700  | 0.39061100  |
| C | -2.72711800 | -0.67581300 | -0.43616900 |
| C | -3.15192900 | -2.01536000 | -0.23251100 |
| C | -4.47207600 | -2.35698000 | -0.60255500 |
| C | -5.31919600 | -1.45855800 | -1.22753000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.85033800 | -0.16416700 | -1.54020700 |
| C | -3.58030900 | 0.20454800  | -1.13637800 |
| C | -0.78465300 | -2.66515500 | 0.04718500  |
| C | 0.20599300  | -3.67068700 | 0.16186700  |
| C | -0.14745800 | -4.93284900 | 0.65938800  |
| C | -1.46547800 | -5.22223800 | 0.98671400  |
| C | -2.48885600 | -4.28965200 | 0.70240800  |
| C | -2.16431900 | -3.00988500 | 0.21199300  |
| H | 0.62576300  | -5.66808100 | 0.83924300  |
| C | 1.93186000  | -2.02474800 | -0.51173500 |
| C | 3.15818000  | -1.77952000 | -1.17044000 |
| C | 4.02486900  | -2.79350600 | -1.52267000 |
| C | 3.67131100  | -4.14144600 | -1.25446000 |
| C | 2.44272000  | -4.40957900 | -0.67142100 |
| C | 1.55421500  | -3.37139200 | -0.30868700 |
| H | 2.12434200  | -5.43705500 | -0.55297200 |
| O | 1.88400200  | 6.59168600  | -1.37288100 |
| O | 6.62616100  | 2.08332100  | 1.53877200  |
| C | 7.69043600  | 1.52242500  | 0.76571400  |
| H | 7.72988500  | 0.43271600  | 0.87072700  |
| H | 7.57936600  | 1.78334400  | -0.29503600 |
| H | 8.61284000  | 1.96320300  | 1.15163400  |
| O | 5.75818900  | -0.58090100 | 2.08780800  |
| C | 6.07632700  | -0.29542500 | 3.45517600  |
| H | 5.16691000  | -0.29479100 | 4.06989500  |
| H | 6.73721400  | -1.09951500 | 3.78768500  |
| H | 6.58472200  | 0.66885400  | 3.55289100  |
| O | 5.18214700  | -2.48495700 | -2.19548600 |
| C | 6.38282500  | -2.64880100 | -1.43372300 |
| H | 6.33954000  | -2.06538100 | -0.50475600 |
| H | 6.56314500  | -3.70254000 | -1.19608300 |
| H | 7.19291100  | -2.27429800 | -2.06437400 |
| O | 4.57396000  | -5.08511400 | -1.65073100 |
| C | 4.24356700  | -6.45000000 | -1.45599600 |
| H | 4.08638200  | -6.67995300 | -0.39348600 |
| H | 3.34560100  | -6.73086300 | -2.02208600 |
| H | 5.09687800  | -7.02033100 | -1.82750300 |
| O | -1.86773400 | -6.38789100 | 1.57873200  |
| C | -0.87783800 | -7.34084000 | 1.92969300  |
| H | -0.35496600 | -7.72854800 | 1.04501900  |
| H | -0.14281400 | -6.91816700 | 2.62674800  |
| H | -1.41164800 | -8.15798300 | 2.41845500  |
| O | -3.79085100 | -4.60142800 | 1.01148900  |
| C | -4.37528400 | -5.72473700 | 0.33962200  |
| H | -4.24361300 | -5.64413600 | -0.74709200 |
| H | -3.94922400 | -6.66635400 | 0.69143800  |
| H | -5.44149700 | -5.68868200 | 0.57662300  |
| O | -6.57597400 | -1.88377800 | -1.60574600 |
| C | -7.65606500 | -1.24015100 | -0.92303700 |
| H | -7.60738000 | -1.44280000 | 0.15534300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -7.64888600 | -0.15854400 | -1.09311300 |
| H | -8.57391300 | -1.67190000 | -1.32937600 |
| O | -4.45894500 | 5.26040700  | 1.77593200  |
| C | -5.74373100 | 5.34318800  | 1.15418600  |
| H | -5.64345500 | 5.44383200  | 0.06502200  |
| H | -6.35980100 | 4.46968700  | 1.38597100  |
| H | -6.21470100 | 6.24259200  | 1.55796900  |
| H | 3.34037700  | -1.04720400 | 1.38621600  |
| H | 3.45368200  | -0.77161000 | -1.42932300 |
| H | -0.61861300 | 5.84639900  | -0.64789600 |
| O | 3.77807100  | 4.81083600  | -0.94910200 |
| C | 4.14095900  | 4.74287300  | -2.33052200 |
| H | 5.18580000  | 5.05745900  | -2.38657000 |
| H | 4.04684300  | 3.71776700  | -2.71116000 |
| H | 3.52413800  | 5.41895300  | -2.93226500 |
| H | -2.20448700 | 5.55649000  | 0.64666400  |
| O | -5.14334500 | 2.66650900  | 2.35028400  |
| C | -5.49407100 | 1.33210600  | 2.68918600  |
| H | -6.44267600 | 1.40171000  | 3.22481600  |
| H | -5.62150900 | 0.70954700  | 1.79451700  |
| H | -4.74080700 | 0.87399700  | 3.34281900  |
| C | 0.92106600  | 7.61971100  | -1.54103300 |
| H | 0.45605400  | 7.89598400  | -0.58573200 |
| H | 1.46809100  | 8.47740100  | -1.93679300 |
| H | 0.13697600  | 7.32873800  | -2.25277200 |
| H | -4.85401000 | -3.34879000 | -0.42612200 |
| O | -5.63422500 | 0.74844800  | -2.21315700 |
| C | -5.88221900 | 0.42530900  | -3.58629400 |
| H | -6.40201800 | -0.53336300 | -3.68343900 |
| H | -6.51002000 | 1.22886700  | -3.97858100 |
| H | -4.94129900 | 0.39069000  | -4.15053600 |
| H | -3.24412500 | 1.20042200  | -1.39494700 |
| H | -3.34673400 | 0.83756800  | 1.50160700  |

## 2d

0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.15597200  | -5.18787000 | -0.46440200 |
| C | 0.53997600  | -3.83680600 | -0.22133300 |
| C | -0.53728300 | -2.90834100 | -0.04320800 |
| C | -1.87805600 | -3.36872100 | 0.15316600  |
| C | -2.02928900 | -4.74813500 | 0.47004500  |
| C | -1.06590200 | -5.63888800 | 0.02342900  |
| C | -0.27426500 | -1.48337300 | -0.05584600 |
| C | -1.35841100 | -0.55415000 | -0.07192100 |
| C | -2.72351300 | -1.03448400 | -0.04903600 |
| C | -2.97833600 | -2.43494100 | 0.01461800  |
| C | 1.91307800  | -3.36117000 | -0.12972800 |
| C | 2.17039300  | -1.94925200 | -0.08340700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.07033700  | -1.00701800 | -0.04564600 |
| C | -3.80417600 | -0.09788600 | -0.06705300 |
| C | -5.09251100 | -0.60546300 | 0.22553400  |
| C | -5.36253200 | -1.95826000 | 0.06524900  |
| C | -4.32390300 | -2.85368500 | -0.18077300 |
| C | 3.04788600  | -4.20274700 | -0.00308100 |
| C | 4.32517000  | -3.71666400 | -0.27233300 |
| C | 4.53892100  | -2.35700300 | -0.44711300 |
| C | 3.50439200  | -1.44953500 | -0.09485600 |
| C | 3.75485500  | -0.04682400 | 0.15097800  |
| C | 2.68620000  | 0.88901200  | 0.07749100  |
| C | 1.32699400  | 0.39852400  | -0.01092700 |
| C | 0.24443300  | 1.32425000  | -0.06303000 |
| C | -1.09771500 | 0.84879500  | -0.11734700 |
| C | -2.19503600 | 1.78931700  | -0.22303600 |
| C | -3.52853800 | 1.30353100  | -0.30709600 |
| C | 5.02386800  | 0.45911000  | 0.52908700  |
| C | 5.32092400  | 1.80133100  | 0.30479800  |
| C | 4.30200100  | 2.68421800  | -0.05588900 |
| C | 2.94535900  | 2.29248600  | 0.09004700  |
| C | 1.83908000  | 3.22436000  | 0.12500600  |
| C | 0.50917200  | 2.74867300  | -0.06225700 |
| C | -0.56413300 | 3.66478900  | -0.25012500 |
| C | -1.93217800 | 3.19581300  | -0.22452700 |
| C | -3.05439600 | 4.04611900  | -0.10050400 |
| C | -4.32390900 | 3.58729800  | -0.44743300 |
| C | -4.53456600 | 2.23292000  | -0.68748200 |
| C | 1.97732200  | 4.61119100  | 0.39945700  |
| C | 1.00775600  | 5.50371700  | -0.06006300 |
| C | -0.21181100 | 5.00991000  | -0.52350300 |
| H | -1.26460300 | -6.70514300 | 0.05378800  |
| H | -6.39322900 | -2.28052900 | 0.14762200  |
| H | 5.12925500  | -4.44043400 | -0.31967000 |
| H | 6.33657500  | 2.15702900  | 0.40321400  |
| H | -5.12338300 | 4.31264400  | -0.54187600 |
| H | 1.20343400  | 6.56697000  | -0.06950600 |
| O | -2.93857100 | 5.34800400  | 0.35111000  |
| C | -3.53514500 | 5.56119100  | 1.62754400  |
| H | -4.61240100 | 5.34859000  | 1.62226200  |
| H | -3.05629000 | 4.94115800  | 2.39749100  |
| H | -3.38073200 | 6.61718300  | 1.86478800  |
| O | -5.65237400 | 1.74696600  | -1.28313800 |
| C | -6.75586300 | 2.61067700  | -1.47691300 |
| H | -7.12758300 | 3.01126500  | -0.52438100 |
| H | -6.50437200 | 3.44493700  | -2.14590100 |
| H | -7.53467000 | 2.00018700  | -1.93707100 |
| O | -6.15030000 | 0.16366600  | 0.66269700  |
| C | -5.97041600 | 0.72453900  | 1.96123400  |
| H | -5.79675100 | -0.06116600 | 2.70954600  |
| H | -5.13812400 | 1.43734100  | 1.98833200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.90095300 | 1.24725800  | 2.19837200  |
| O | -4.53803000 | -4.13260500 | -0.57707100 |
| C | -5.86813100 | -4.60031300 | -0.70762700 |
| H | -6.39578600 | -4.59861000 | 0.25551800  |
| H | -6.43640900 | -3.99941600 | -1.42982500 |
| H | -5.78557500 | -5.62676100 | -1.06858800 |
| O | -3.07450600 | -5.31839200 | 1.14731300  |
| C | -3.51026500 | -4.66886300 | 2.33655400  |
| H | -2.65633200 | -4.38696200 | 2.96553400  |
| H | -4.11096300 | -3.77622200 | 2.13241900  |
| H | -4.12396600 | -5.40143800 | 2.86736500  |
| O | 0.91318800  | -6.15801600 | -1.05911200 |
| C | 1.54344600  | -5.83322100 | -2.29479400 |
| H | 0.82034300  | -5.39075900 | -2.99156800 |
| H | 2.38882300  | -5.15149500 | -2.16853200 |
| H | 1.90580200  | -6.78142200 | -2.69844400 |
| O | 3.01024900  | -5.54288000 | 0.29556700  |
| C | 2.51463200  | -5.88130800 | 1.58887400  |
| H | 3.14562900  | -5.43802900 | 2.37118300  |
| H | 1.47861500  | -5.55936700 | 1.73322000  |
| H | 2.56259000  | -6.97052600 | 1.65273300  |
| O | 5.69877700  | -1.85227500 | -0.94991800 |
| C | 6.73700100  | -2.75648800 | -1.27918300 |
| H | 7.12884800  | -3.26760000 | -0.38939800 |
| H | 6.40274000  | -3.50913800 | -2.00552800 |
| H | 7.52935200  | -2.15165400 | -1.72514400 |
| O | 5.90111000  | -0.39699800 | 1.11978800  |
| C | 7.21871100  | 0.04678700  | 1.37718300  |
| H | 7.74631100  | 0.31114700  | 0.45048700  |
| H | 7.23118700  | 0.90933800  | 2.05741200  |
| H | 7.72915700  | -0.79188000 | 1.85519400  |
| O | 4.56663800  | 3.91776100  | -0.56732100 |
| C | 5.91357700  | 4.32550500  | -0.70578600 |
| H | 6.41160200  | 4.42906100  | 0.26831800  |
| H | 6.48687400  | 3.62677200  | -1.32979600 |
| H | 5.88104400  | 5.30099700  | -1.19561600 |
| O | 3.05668500  | 5.01463100  | 1.12175000  |
| C | 3.28662100  | 6.39986600  | 1.28762300  |
| H | 3.46786500  | 6.89956000  | 0.32613800  |
| H | 2.44673300  | 6.89263200  | 1.79603600  |
| H | 4.17995200  | 6.48281800  | 1.91021500  |
| O | -1.07648600 | 5.75300300  | -1.25845500 |
| C | -0.94375900 | 7.16085500  | -1.26181000 |
| H | -0.99318500 | 7.56966300  | -0.24431700 |
| H | -0.00604700 | 7.47924800  | -1.73810300 |
| H | -1.78663700 | 7.53959800  | -1.84270500 |

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|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.94469700  | 1.44705900  | 0.11105700  |
| C | 3.53614700  | 1.46807200  | 0.06339800  |
| C | 2.85118700  | 0.23865600  | -0.14599100 |
| C | 3.59041200  | -0.98130000 | -0.29107400 |
| C | 4.96444600  | -0.97363300 | 0.00056000  |
| C | 5.64569600  | 0.25224600  | 0.11825200  |
| C | 1.40766600  | 0.19496100  | -0.12866800 |
| C | 0.74153600  | -1.05717800 | -0.12322100 |
| C | 1.48400000  | -2.27542500 | -0.32080400 |
| C | 2.87616400  | -2.21954300 | -0.61588000 |
| C | 2.76573000  | 2.71132600  | 0.21584200  |
| C | 1.33750700  | 2.65986900  | 0.06186300  |
| C | 0.65667700  | 1.39368700  | -0.04948200 |
| C | 0.81718300  | -3.52137700 | -0.32163100 |
| C | 1.49283500  | -4.65578800 | -0.79990800 |
| C | 2.76616100  | -4.54560000 | -1.34335900 |
| C | 3.47384600  | -3.31999100 | -1.26664700 |
| C | 3.34925000  | 3.96222000  | 0.51493800  |
| C | 2.56918300  | 5.13279800  | 0.58191300  |
| C | 1.20327600  | 5.07583000  | 0.36419800  |
| C | 0.56976200  | 3.85212500  | 0.10249400  |
| C | -0.87212600 | 3.80032300  | -0.12764500 |
| C | -1.54677700 | 2.55251600  | -0.11937600 |
| C | -0.77148300 | 1.33935200  | -0.03722300 |
| C | -1.42924200 | 0.08569400  | 0.01851300  |
| C | -0.67011900 | -1.11204600 | -0.01012500 |
| C | -1.31910300 | -2.38611200 | 0.16523300  |
| C | -0.56002500 | -3.58044700 | 0.14461000  |
| C | -1.59700600 | 4.97906700  | -0.35647400 |
| C | -2.96326300 | 4.93691900  | -0.57568100 |
| C | -3.65144800 | 3.70864300  | -0.54507800 |
| C | -2.97482100 | 2.49797400  | -0.27769700 |
| C | -3.64595500 | 1.19616500  | -0.15630200 |
| C | -2.87181700 | 0.01954500  | 0.03330500  |
| C | -3.52157200 | -1.24886200 | 0.17707900  |
| C | -2.70813700 | -2.43113200 | 0.48025000  |
| C | -3.20435200 | -3.59157100 | 1.09884700  |
| C | -2.43119300 | -4.77365900 | 1.11416600  |
| C | -1.14696400 | -4.77848500 | 0.58331400  |
| C | -5.04644700 | 1.05880800  | -0.23210800 |
| C | -5.65764000 | -0.18309300 | -0.27332000 |
| C | -4.89532700 | -1.36142000 | -0.12372900 |
| O | -4.42572900 | -3.60116300 | 1.73174200  |
| C | -4.33842100 | -3.57523100 | 3.15806000  |
| H | -3.84806700 | -4.47390300 | 3.54708100  |
| H | -3.79970700 | -2.68229100 | 3.50098900  |
| H | -5.36821100 | -3.53841600 | 3.52285800  |
| O | 4.63279800  | -3.12016300 | -1.94725900 |
| C | 5.70871000  | -4.06039400 | -1.87332200 |
| H | 5.72837000  | -4.57179800 | -0.90737300 |

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|---|-------------|-------------|-------------|
| H | 5.62990200  | -4.79821800 | -2.67582400 |
| H | 6.62359600  | -3.47483300 | -1.98445800 |
| O | 5.66140000  | -2.14231900 | 0.18631700  |
| C | 6.09353200  | -2.36298200 | 1.53115300  |
| H | 6.81013100  | -1.60143800 | 1.85378400  |
| H | 5.23694600  | -2.38183400 | 2.21747200  |
| H | 6.57889400  | -3.34231000 | 1.53332600  |
| O | 4.70146000  | 4.12874800  | 0.74312400  |
| C | 5.05629100  | 4.22529900  | 2.12636500  |
| H | 4.55754600  | 5.07643200  | 2.60009000  |
| H | 4.80522000  | 3.30065000  | 2.66146600  |
| H | 6.13802400  | 4.38066700  | 2.15318300  |
| O | -5.01191200 | 3.77685300  | -0.77592900 |
| C | -5.36685100 | 3.89256700  | -2.15822600 |
| H | -4.93608700 | 4.79692300  | -2.59863500 |
| H | -5.03932000 | 3.01035400  | -2.72269000 |
| H | -6.45743500 | 3.96160100  | -2.18766000 |
| O | -5.40233000 | -2.58869800 | -0.40600200 |
| C | -6.66363200 | -3.01537000 | 0.11919200  |
| H | -6.85039000 | -2.58677600 | 1.10719500  |
| H | -7.47622400 | -2.74170700 | -0.55812600 |
| H | -6.59211500 | -4.10085700 | 0.21017100  |
| O | -6.99845300 | -0.35590100 | -0.49830700 |
| H | -5.64690900 | 1.94709100  | -0.31343800 |
| C | -7.80716100 | 0.79406700  | -0.67520200 |
| H | -7.79508800 | 1.44100000  | 0.21160200  |
| H | -7.49092800 | 1.37947000  | -1.54860200 |
| H | -8.82097200 | 0.42197000  | -0.83717300 |
| H | -0.55655900 | -5.68547400 | 0.60034000  |
| O | -3.03393500 | -5.85874800 | 1.69007500  |
| C | -2.31793200 | -7.08100600 | 1.72156400  |
| H | -2.07496600 | -7.43249500 | 0.70988000  |
| H | -1.39042900 | -6.99482700 | 2.30388500  |
| H | -2.98065800 | -7.80280000 | 2.20304900  |
| H | 0.96415600  | -5.59829700 | -0.86106700 |
| O | 3.40024200  | -5.56262600 | -2.00625500 |
| C | 2.71546400  | -6.79191200 | -2.16810500 |
| H | 2.49585500  | -7.26551300 | -1.20148600 |
| H | 1.77855700  | -6.66158400 | -2.72564700 |
| H | 3.38869100  | -7.43564600 | -2.73771900 |
| H | 5.47536000  | 2.38015600  | 0.17560400  |
| O | 7.00526700  | 0.16077200  | 0.25424000  |
| C | 7.75058300  | 1.36460400  | 0.33269000  |
| H | 7.61420500  | 1.98295500  | -0.56358500 |
| H | 7.47834200  | 1.95488900  | 1.21799300  |
| H | 8.79691400  | 1.06154700  | 0.40763100  |
| H | 0.61743600  | 5.97910400  | 0.45163900  |
| O | 3.25487900  | 6.27804700  | 0.88085300  |
| C | 2.53381100  | 7.49686500  | 0.92947500  |
| H | 2.05253000  | 7.71972700  | -0.03214000 |

|   |             |            |             |
|---|-------------|------------|-------------|
| H | 1.77122200  | 7.48882800 | 1.72020000  |
| H | 3.27185600  | 8.27055400 | 1.14990200  |
| H | -1.08210000 | 5.92654800 | -0.41860100 |
| O | -3.73450600 | 6.03469300 | -0.84288800 |
| C | -3.10759600 | 7.30528500 | -0.86113500 |
| H | -2.64283900 | 7.54010600 | 0.10579300  |
| H | -2.34793300 | 7.37431600 | -1.65165700 |
| H | -3.90231300 | 8.02626000 | -1.06244900 |