

## On the Simulation of Vibrationally Resolved Electronic Spectra of medium-size molecules: the case of Styryl Substituted Bodipys

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




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**Table S1.** Wavelength corresponding to the vertical excitation energies for **mono-bdp** system, computed by using several basis sets and two different density functionals.

|                                 | CAM-B3LYP   |              | $\omega$ B97XD |      |
|---------------------------------|-------------|--------------|----------------|------|
|                                 | 6-311G(d,p) | 6-311+G(d,p) | 6-311G(d,p)    | SNSD |
| Vertical excitation energy (nm) | 478         | 483          | 474            | 482  |
| Transition dipole moment (D)    | 5.34        | 5.45         | 5.33           | 5.39 |

**Table S2.** Comparison between colors, expressed with the RGB model, simulated using normalized experimental spectra and computed at the TD AH|FCHT spectra with all ten functionals, for mono-bdp and bis-bdp system and their absorption and emission process. All the colors have been simulated using the VMS draw program, in which the color system used is SMPTE C and the reference for white is  $x_n=0.312713$ ;  $y_n=0.329016$ .

|                                 | mono-bdp (Abs)           |   | mono-bdp (Emi)         |   | bis-bdp (Abs)          |   | bis-bdp (Emi)         |   |
|---------------------------------|--------------------------|---|------------------------|---|------------------------|---|-----------------------|---|
| <b>exp</b>                      | R:73<br>G:145<br>B:247   |   | R:0<br>G:243<br>B:255  |   | R:65<br>G:239<br>B:162 |   | R:0<br>G:255<br>B:194 |   |
| <b>B3LYP-D3</b>                 | R: 104<br>G:152<br>B:225 |  | R:0<br>G:255<br>B:223  |  | R:0<br>G:203<br>B:255  |  | R:0<br>G:255<br>B:0   |  |
| <b>B3LYP</b>                    | R:85<br>G:158<br>B:228   |  | R:0<br>G:255<br>B:220  |  | R:0<br>G:202<br>B:255  |  | R:0<br>G:255<br>B:0   |  |
| <b>CAM-B3LYP-D3</b>             | R:255<br>G:2<br>B:156    |  | R:0<br>G:156<br>B:255  |  | R:0<br>B:203<br>G:255  |  | R:0<br>G:255<br>B:192 |  |
| <b>CAM-B3LYP</b>                | R:255<br>G:8<br>B:160    |  | R:0<br>G:158<br>B:255  |  | R:0<br>G:193<br>B:255  |  | R:0<br>G:255<br>B:192 |  |
| <b>M062X</b>                    | R:255<br>G:22<br>B:203   |  | R:0<br>G:163<br>B:255  |  | R:0<br>G:199<br>B:255  |  | R:0<br>G:255<br>B:191 |  |
| <b>MN15</b>                     | R:148<br>G:100<br>B: 252 |  | R:0<br>G:224<br>B:255  |  | R:28<br>G:165<br>B:250 |  | R:0<br>G:255<br>B:185 |  |
| <b>PBE0</b>                     | R:158<br>G:141<br>B:208  |  | R:0<br>G:255<br>B:245  |  | R:0<br>G:184<br>B:255  |  | R:0<br>G:255<br>B:59  |  |
| <b>PBE0-D3</b>                  | R:144<br>G:138<br>B:217  |  | R:0<br>G:255<br>B:247  |  | R:0<br>G:184<br>B:255  |  | R:0<br>G:255<br>B:65  |  |
| <b><math>\omega</math>B97X</b>  | R:255<br>G:0<br>B:80     |  | R:30<br>G:112<br>B:255 |  | R:64<br>G:162<br>B:235 |  | R:0<br>G:255<br>B:199 |  |
| <b><math>\omega</math>B97XD</b> | R:255<br>G:0<br>B:160    |  | R:0<br>G:151<br>B:255  |  | R:0<br>G:195<br>B:255  |  | R:0<br>G:255<br>B:193 |  |

**Table S3.** Stoke shift, vertical excitation and emission energies of **mono-bdp** and **bis-bdp** in methanol computed with the NEQ-LR-PCM and EQ-SS-PCM approaches respectively, using maximum bands of the spectra and by using the NEQ-SS-PCM and EQ-SS-PCM approaches respectively, along with experimental values.

|                                 | <b>mono-bdp</b>       |                    |             |
|---------------------------------|-----------------------|--------------------|-------------|
|                                 | absorption/NEQ-LR-PCM | emission/EQ-SS-PCM | Stoke Shift |
| <b>exp values</b>               | 596                   | 605                | 9           |
| <b>CAM-B3LYP</b>                | 478.2                 | 504.3              | 26.1        |
| <b>CAM-B3LYP-D3</b>             | 476.9                 | 502.6              | 25.7        |
| <b>PBE0</b>                     | 509.1                 | 536.6              | 27.5        |
| <b>PBE0</b>                     | 508                   | 535.1              | 27.1        |
| <b>B3LYP</b>                    | 522.5                 | 551.4              | 28.9        |
| <b>B3LYP-D3</b>                 | 520.3                 | 549.1              | 28.8        |
| <b><math>\omega</math>B97X</b>  | 466.8                 | 488.9              | 22.1        |
| <b><math>\omega</math>B97XD</b> | 473.2                 | 496.9              | 23.7        |
| <b>M06-2X</b>                   | 482.9                 | 508.2              | 25.3        |
| <b>MN15</b>                     | 498.6                 | 523.8              | 25.2        |

|                                 | <b>mono-bdp</b>     |                   |             |
|---------------------------------|---------------------|-------------------|-------------|
|                                 | absorption/spectrum | emission/spectrum | Stoke Shift |
| <b>exp values</b>               | 596                 | 605               | 9           |
| <b>CAM-B3LYP</b>                | 565                 | 570               | 5           |
| <b>CAM-B3LYP-D3</b>             | 563                 | 570               | 7           |
| <b>PBE0</b>                     | 604                 | 610               | 6           |
| <b>PBE0</b>                     | 602                 | 610               | 8           |
| <b>B3LYP</b>                    | 620                 | 625               | 5           |
| <b>B3LYP-D3</b>                 | 615                 | 623               | 8           |
| <b><math>\omega</math>B97X</b>  | 550                 | 550               | 0           |
| <b><math>\omega</math>B97XD</b> | 560                 | 567               | 7           |
| <b>M06-2X</b>                   | 568                 | 573               | 5           |
| <b>MN15</b>                     | 590                 | 595               | 5           |

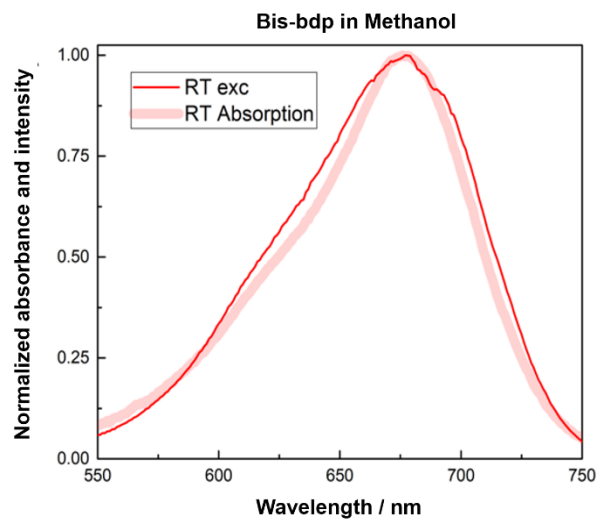
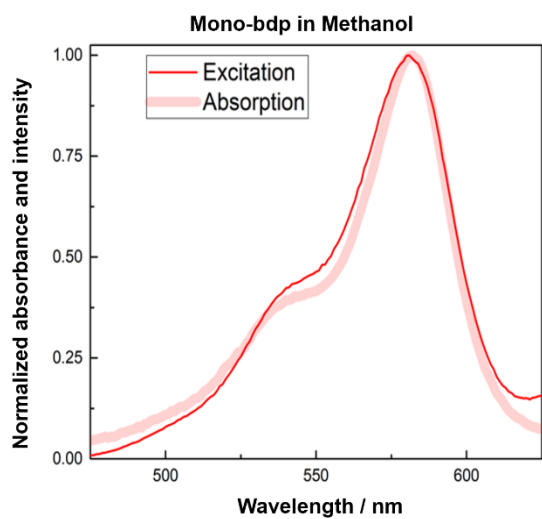
|                                 | <b>mono-bdp</b>       |                    |             |
|---------------------------------|-----------------------|--------------------|-------------|
|                                 | absorption/NEQ-SS-PCM | emission/EQ-SS-PCM | Stoke Shift |
| <b>exp values</b>               | 596                   | 605                | 9           |
| <b>CAM-B3LYP</b>                | 481                   | 504.3              | 23.3        |
| <b>CAM-B3LYP-D3</b>             | 451.1                 | 502.6              | 51.5        |
| <b>PBE0</b>                     | 485.9                 | 536.6              | 50.7        |
| <b>PBE0</b>                     | 484.3                 | 535.1              | 50.8        |
| <b>B3LYP</b>                    | 500.6                 | 551.4              | 50.8        |
| <b>B3LYP-D3</b>                 | 498.6                 | 549.1              | 50.5        |
| <b><math>\omega</math>B97X</b>  | 440.5                 | 488.9              | 48.4        |
| <b><math>\omega</math>B97XD</b> | 447.3                 | 496.9              | 49.6        |
| <b>M06-2X</b>                   | 457.1                 | 508.2              | 51.1        |
| <b>MN15</b>                     | 472.3                 | 523.8              | 51.5        |

|  | <b>bis-bdp</b>        |                    |             |
|--|-----------------------|--------------------|-------------|
|  | absorption/NEQ-LR-PCM | emission/EQ-SS-PCM | Stoke Shift |

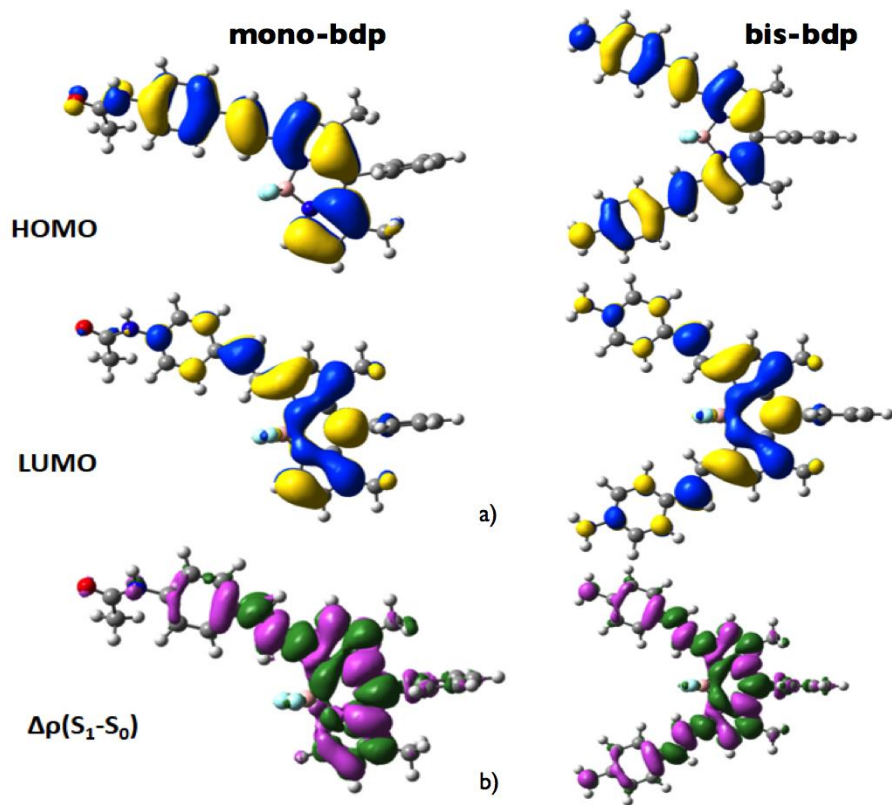
|                |       |       |      |
|----------------|-------|-------|------|
| exp values     | 729   | 751   | 22   |
| CAM-B3LYP      | 572.5 | 624.6 | 52.1 |
| CAM-B3LYP-D3   | 573.4 | 623.4 | 50   |
| PBE0           | 640.5 | 673.5 | 33   |
| PBE0           | 640.6 | 673.8 | 31.2 |
| B3LYP          | 660.7 | 690.3 | 29.6 |
| B3LYP-D3       | 660.4 | 689.2 | 28.8 |
| $\omega$ B97X  | 541.9 | 590.4 | 48.5 |
| $\omega$ B97XD | 561.9 | 609.9 | 48   |
| M06-2X         | 580.4 | 633.3 | 52.9 |
| MN15           | 612.2 | 662.4 | 50.2 |

|                | bis-bdp             |                   |             |
|----------------|---------------------|-------------------|-------------|
|                | absorption/spectrum | emission/spectrum | Stoke Shift |
| exp values     | 729                 | 751               | 22          |
| CAM-B3LYP      | 695                 | 700               | 5           |
| CAM-B3LYP-D3   | 697                 | 700               | 3           |
| PBE0           | 782                 | 785               | 3           |
| PBE0           | 782                 | 785               | 3           |
| B3LYP          | 806                 | 810               | 4           |
| B3LYP-D3       | 806                 | 810               | 4           |
| $\omega$ B97X  | 652                 | 658               | 6           |
| $\omega$ B97XD | 681                 | 684               | 3           |
| M06-2X         | 705                 | 753               | 48          |
| MN15           | 720                 | 751               | 31          |

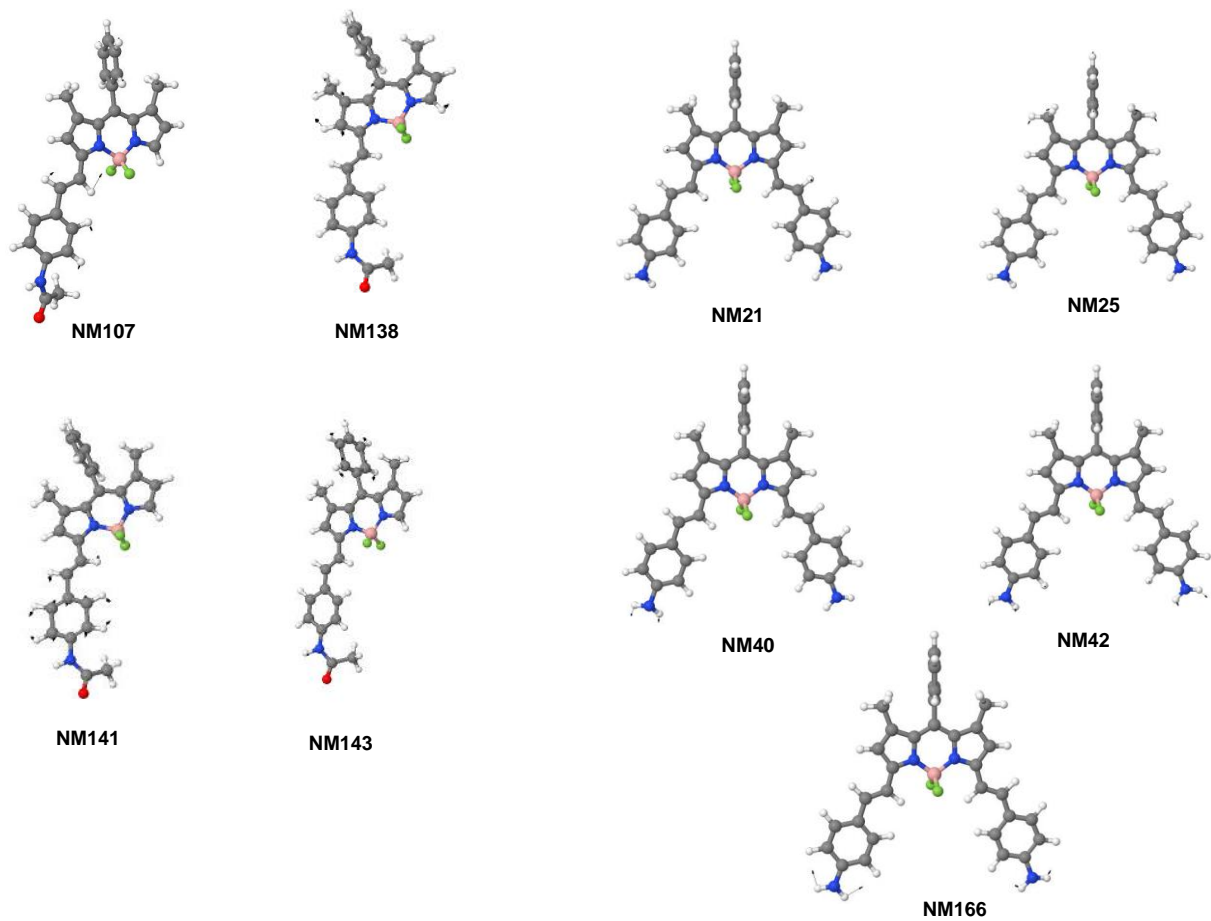
|                | bis-bdp              |                    |             |
|----------------|----------------------|--------------------|-------------|
|                | absorption/EQ-SS-PCM | emission/EQ-SS-PCM | Stoke Shift |
| exp values     | 729                  | 751                | 22          |
| CAM-B3LYP      | 546.9                | 624.6              | 77.7        |
| CAM-B3LYP-D3   | 547.7                | 623.4              | 75.7        |
| PBE0           | 618.6                | 673.5              | 54.9        |
| PBE0           | 618.6                | 673.8              | 55.2        |
| B3LYP          | 638.5                | 690.3              | 51.8        |
| B3LYP-D3       | 637.8                | 689.2              | 51.4        |
| $\omega$ B97X  | 514.2                | 590.4              | 76.2        |
| $\omega$ B97XD | 535                  | 609.9              | 74.9        |
| M06-2X         | 556.3                | 633.3              | 77          |
| MN15           | 589                  | 662.4              | 73.4        |



**Figure S1.** Comparison between the absorption and excitation spectra of (left) **mono-bdp** and (right) **bis-bdp** molecules.



**Figure S2.** a) Highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals of **mono-bdp** and **bis-bdp**. b) Electron density change ( $\Delta\rho_{S_1-S_0}$ ) of mono-bdp and bis-bdp.



**Figure S3** Representation of the normal modes (NM) giving significant contributions in the OPA and OPE spectra of **mono-bdp** and **bis-bdp**.

Example of G16 input file for computing vibronic spectra with reduced dimensionality in Cartesian coordinates.

```
%NProcShared=10
%Mem=12GB
%OldChk=bodipy_A.S0.frq.chk
#P Geom=Check Freq=(ReadFC,ReadNM,ReadFCHT)

bodipy_A / MN15.6-311G_d_p_ : OPA TD AH|FC Cart

0 1

OPA TD AH FC
Print=(Matrix=JKC)
Spectrum=(Lower=-6000,Upper=+24000,HWHM=250.)
RedDim=(ClearLowFreq=50,BlockThresh=.6)

bodipy_A.S1.frq.chk
```

Cartesian Coordinates for the optimized structures of **mono-bdp** and **bis-bdp** systems in both the ground and excited states, computed at MN15/6-311G(d,p) level of theory:

#### mono-bdp S0

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 8.09711600  | 2.45453400  | 0.11353400  |
| C | 6.05398700  | -1.08364400 | -0.52503200 |
| C | 7.08812100  | -2.02112700 | -0.49011100 |
| C | 8.28390900  | -1.32702700 | -0.29568500 |
| H | 4.99205900  | -1.23788600 | -0.65056000 |
| H | 6.98113700  | -3.09107000 | -0.58713400 |
| C | 6.40025500  | 3.89832800  | 0.11576200  |
| C | 8.65606500  | 3.76195200  | 0.30440300  |
| C | 7.59312100  | 4.64101200  | 0.30615400  |
| H | 7.65996900  | 5.71142900  | 0.43205100  |
| B | 5.72425400  | 1.44770500  | -0.32583100 |
| F | 4.72979600  | 1.35209000  | 0.65774200  |
| F | 5.11018100  | 1.68297800  | -1.56308000 |
| N | 6.55296400  | 0.15128800  | -0.36502800 |
| N | 6.71483400  | 2.59273400  | 0.00180300  |
| C | 9.63099500  | -1.97291600 | -0.18830400 |
| H | 10.24461000 | -1.77299700 | -1.07058300 |
| H | 10.19326200 | -1.61360500 | 0.67666400  |
| H | 9.51048300  | -3.05359800 | -0.09900900 |
| C | 10.08875800 | 4.16216100  | 0.46873900  |
| H | 10.48391400 | 3.84546000  | 1.43696800  |
| H | 10.72819600 | 3.71641000  | -0.29641300 |
| H | 10.17265400 | 5.24787800  | 0.40564100  |
| C | 10.17371800 | 1.07636700  | 0.15249000  |
| C | 10.75364600 | 1.08797300  | 1.42146400  |
| C | 10.97532700 | 0.93289000  | -0.98046700 |
| C | 12.13235400 | 0.95327700  | 1.55616000  |
| H | 10.12197300 | 1.20020900  | 2.29647600  |
| C | 12.35498200 | 0.81017400  | -0.84352500 |
| H | 10.51476300 | 0.91917600  | -1.96275100 |
| C | 12.93367300 | 0.81736800  | 0.42418800  |
| H | 12.58064600 | 0.95767000  | 2.54271800  |
| H | 12.97683600 | 0.70506500  | -1.72472900 |
| H | 14.00751000 | 0.71685500  | 0.52972800  |
| C | 5.03396700  | 4.36276000  | 0.03785800  |
| H | 4.27477000  | 3.59469300  | -0.05477300 |
| C | 4.69923200  | 5.66742100  | 0.07734800  |
| H | 5.49275900  | 6.40700600  | 0.16090600  |



|   |             |            |             |
|---|-------------|------------|-------------|
| C | 3.34968700  | 6.22116100 | 0.01321900  |
| C | 3.19045200  | 7.61480400 | 0.01664500  |
| C | 2.19169000  | 5.42896600 | -0.03797800 |
| C | 1.93424900  | 8.19661100 | -0.05585700 |
| H | 4.07035600  | 8.24752000 | 0.06555600  |
| C | 0.93244500  | 6.00327300 | -0.08850500 |
| H | 2.26815500  | 4.34826200 | -0.01121300 |
| C | 0.79078100  | 7.39620600 | -0.12138900 |
| H | 1.82910600  | 9.27564000 | -0.06987700 |
| H | 0.05421700  | 5.37082900 | -0.07542500 |
| N | -0.47181900 | 8.02233200 | -0.15462900 |
| H | -0.56307900 | 8.89029500 | 0.36415500  |
| C | -1.59581300 | 7.72376600 | -0.88800200 |
| O | -2.60011600 | 8.40697300 | -0.75461800 |
| C | -1.54393500 | 6.57388100 | -1.86029900 |
| H | -0.55451400 | 6.42963000 | -2.29424200 |
| H | -1.83808800 | 5.64849300 | -1.36020000 |
| H | -2.27157100 | 6.77963300 | -2.64321700 |

**mono-bdp-S1**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 7.92776900  | 0.06141500  | -0.23568600 |
| C | 8.71686900  | 1.20045800  | 0.01053400  |
| C | 8.08830700  | 2.46558400  | 0.10812100  |
| C | 6.03659700  | -1.04929200 | -0.59406200 |
| C | 7.05890800  | -2.00429400 | -0.53071100 |
| C | 8.25798500  | -1.33493600 | -0.30105900 |
| H | 4.97498000  | -1.18653700 | -0.74274000 |
| H | 6.93322300  | -3.07285600 | -0.62733300 |
| C | 6.39488400  | 3.93549900  | 0.10058500  |
| C | 8.66044000  | 3.78410000  | 0.29661800  |
| C | 7.60798300  | 4.66383900  | 0.29371500  |
| H | 7.68420800  | 5.73539600  | 0.41001900  |
| B | 5.73691000  | 1.48108900  | -0.37548500 |
| F | 4.71205600  | 1.37598600  | 0.58251100  |
| F | 5.13799500  | 1.73732600  | -1.62162900 |
| N | 6.55319500  | 0.18170200  | -0.41798400 |
| N | 6.72528100  | 2.59946600  | -0.01154400 |
| C | 9.59017000  | -1.99410300 | -0.13236600 |
| H | 10.23725700 | -1.84083600 | -1.00156900 |
| H | 10.13416200 | -1.60727000 | 0.73362500  |
| H | 9.45124600  | -3.06894900 | -0.00278500 |
| C | 10.09946100 | 4.16881600  | 0.44141700  |
| H | 10.50830900 | 3.86489800  | 1.40852900  |
| H | 10.72556200 | 3.70642000  | -0.32567100 |
| H | 10.19353300 | 5.25286800  | 0.35940400  |
| C | 10.18575800 | 1.06728900  | 0.16175300  |
| C | 10.78096000 | 1.16876100  | 1.42234200  |
| C | 10.98781800 | 0.82257800  | -0.95648100 |
| C | 12.15832100 | 1.02721400  | 1.56266600  |
| H | 10.15648200 | 1.35411200  | 2.29044500  |
| C | 12.36605200 | 0.68881700  | -0.81752800 |
| H | 10.52298300 | 0.74100500  | -1.93380200 |
| C | 12.95298600 | 0.78918500  | 0.44263200  |
| H | 12.61132600 | 1.10231800  | 2.54447200  |
| H | 12.98133200 | 0.50543800  | -1.69081200 |
| H | 14.02595100 | 0.68177100  | 0.55154500  |
| C | 5.07247100  | 4.39790300  | 0.01695200  |
| H | 4.30836900  | 3.64180200  | -0.12503900 |
| C | 4.71173700  | 5.72979300  | 0.10931700  |
| H | 5.49784300  | 6.46786600  | 0.25105700  |
| C | 3.38429300  | 6.24697500  | 0.03374300  |
| C | 3.18193500  | 7.64640000  | 0.13978700  |
| C | 2.23110300  | 5.43826900  | -0.12961300 |

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 1.92402400  | 8.19999600 | 0.05910400  |
| H | 4.04369200  | 8.29061800 | 0.27705000  |
| C | 0.96922200  | 5.98890900 | -0.19905200 |
| H | 2.32679600  | 4.36033700 | -0.17733400 |
| C | 0.79451700  | 7.38355200 | -0.13307800 |
| H | 1.79271800  | 9.27428200 | 0.12792100  |
| H | 0.11038400  | 5.33596800 | -0.27028300 |
| N | -0.45701600 | 8.00016800 | -0.18552300 |
| H | -0.53351800 | 8.89754900 | 0.28529200  |
| C | -1.61426200 | 7.68079600 | -0.87162600 |
| O | -2.60018800 | 8.38256100 | -0.71757000 |
| C | -1.60876500 | 6.51008000 | -1.81666100 |
| H | -0.64445900 | 6.36811500 | -2.30486100 |
| H | -1.86454800 | 5.59249200 | -1.28230900 |
| H | -2.38222700 | 6.69359300 | -2.55998400 |

**bis-bdp S0**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 7.97622900  | -0.10208600 | 0.05614900  |
| C | 8.67134500  | 1.11117700  | 0.05923300  |
| C | 7.98420500  | 2.32893300  | 0.06374500  |
| C | 6.16633600  | -1.40945000 | 0.06344400  |
| C | 7.30514000  | -2.25046100 | 0.08574900  |
| C | 8.43626100  | -1.45560600 | 0.08306000  |
| H | 7.29522400  | -3.33033200 | 0.10529600  |
| C | 6.18278700  | 3.64800800  | 0.05971300  |
| C | 8.45292900  | 3.67947300  | 0.03634800  |
| C | 7.32700800  | 4.48163600  | 0.03576000  |
| H | 7.32412300  | 5.56155400  | 0.01624900  |
| B | 5.67226900  | 1.12094200  | 0.06135500  |
| F | 4.84835400  | 1.11074900  | 1.20067200  |
| F | 4.84783000  | 1.13656100  | -1.07753800 |
| N | 6.58506500  | -0.12243400 | 0.04826200  |
| N | 6.59319500  | 2.35831600  | 0.07400700  |
| C | 9.83975500  | -1.97791500 | 0.10739300  |
| H | 10.35420600 | -1.79288800 | -0.83887600 |
| H | 10.43921500 | -1.50805100 | 0.89040800  |
| H | 9.82424800  | -3.05499500 | 0.28078000  |
| C | 9.85966200  | 4.19286400  | 0.00949900  |
| H | 10.37481300 | 4.00416000  | 0.95465500  |
| H | 10.45454800 | 3.71961100  | -0.77495700 |
| H | 9.85061600  | 5.27010200  | -0.16336600 |
| C | 10.15816000 | 1.10628300  | 0.05753300  |
| C | 10.85920800 | 1.28081600  | 1.25126100  |
| C | 10.85521100 | 0.92711500  | -1.13785800 |
| C | 12.25121300 | 1.27220800  | 1.24945800  |
| H | 10.30993100 | 1.42205400  | 2.17635400  |
| C | 12.24723500 | 0.92646500  | -1.13936200 |
| H | 10.30279300 | 0.78950400  | -2.06162800 |
| C | 12.94595300 | 1.09701700  | 0.05422600  |
| H | 12.79274500 | 1.40448600  | 2.17885600  |
| H | 12.78566900 | 0.79059400  | -2.07004200 |
| H | 14.02970100 | 1.09340000  | 0.05293600  |
| C | 4.78590700  | 4.00870800  | 0.06749500  |
| H | 4.08007900  | 3.18629600  | 0.09372000  |
| C | 4.35528500  | 5.28913100  | 0.04653400  |
| H | 5.10099200  | 6.08217000  | 0.02320700  |
| C | 2.97782300  | 5.75437900  | 0.05194900  |
| C | 2.72371700  | 7.13590400  | 0.03786600  |
| C | 1.86308400  | 4.89532700  | 0.06852500  |
| C | 1.43595600  | 7.64343700  | 0.04136400  |
| H | 3.56433300  | 7.82299100  | 0.02174300  |
| C | 0.57324000  | 5.38878400  | 0.07236900  |
| H | 2.00735400  | 3.82042400  | 0.07536300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.32968100  | 6.77724600  | 0.05942600  |
| H | 1.27062900  | 8.71561700  | 0.03039700  |
| H | -0.26964700 | 4.70552300  | 0.08570100  |
| N | -0.95500000 | 7.26713800  | 0.10725900  |
| H | -1.10054700 | 8.23015900  | -0.16138800 |
| H | -1.70704400 | 6.64279500  | -0.14826000 |
| C | 4.76711300  | -1.76100300 | 0.05714800  |
| H | 4.06674600  | -0.93393100 | 0.03103200  |
| C | 4.32789600  | -3.03847700 | 0.07958000  |
| H | 5.06814900  | -3.83652700 | 0.10551500  |
| C | 2.94726900  | -3.49429200 | 0.07315600  |
| C | 2.68347300  | -4.87386000 | 0.09805800  |
| C | 1.83866900  | -2.62782900 | 0.04048100  |
| C | 1.39224900  | -5.37252200 | 0.09124800  |
| H | 3.51925400  | -5.56664400 | 0.12095000  |
| C | 0.54546900  | -3.11238600 | 0.03387400  |
| H | 1.99041400  | -1.55417600 | 0.01807400  |
| C | 0.29212500  | -4.49891700 | 0.05916600  |
| H | 1.21943900  | -6.44340000 | 0.11091500  |
| H | -0.29245700 | -2.42336000 | 0.00952100  |
| N | -0.99687300 | -4.97846400 | 0.09618400  |
| H | -1.73882700 | -4.35753200 | -0.19474000 |
| H | -1.14392500 | -5.94845000 | -0.14524300 |

**bis-bdp-S1**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 7.99135800  | 2.32701500  | 0.05713500  |
| C | 6.16635400  | -1.41985900 | 0.05742000  |
| C | 7.31466200  | -2.25746200 | 0.09640300  |
| C | 8.44320800  | -1.46898200 | 0.09877500  |
| H | 7.30314000  | -3.33793900 | 0.12516600  |
| C | 6.18148200  | 3.65636500  | 0.05304800  |
| C | 8.45874300  | 3.69203400  | 0.02019300  |
| C | 7.33492400  | 4.48720800  | 0.02132200  |
| H | 7.33004200  | 5.56777600  | -0.00571000 |
| B | 5.69683500  | 1.11966300  | 0.05217900  |
| F | 4.85552300  | 1.10559500  | 1.18760500  |
| F | 4.85988200  | 1.13878200  | -1.08663800 |
| N | 6.60511200  | -0.11477100 | 0.03706900  |
| N | 6.61237100  | 2.34865800  | 0.07076500  |
| C | 9.84874300  | -1.98352900 | 0.14935200  |
| H | 10.38039400 | -1.81484100 | -0.79127600 |
| H | 10.43672600 | -1.49868600 | 0.93290200  |
| H | 9.83541100  | -3.05785000 | 0.34234900  |
| C | 9.86735200  | 4.19858300  | -0.02540400 |
| H | 10.39518100 | 4.02578900  | 0.91662000  |
| H | 10.45493600 | 3.71141000  | -0.80779900 |
| H | 9.86068400  | 5.27321100  | -0.21707200 |
| C | 10.18853000 | 1.10625300  | 0.05980800  |
| C | 10.89574800 | 1.34053800  | 1.24183700  |
| C | 10.89701700 | 0.86768200  | -1.12061200 |
| C | 12.28797300 | 1.33522400  | 1.24509100  |
| H | 10.34527900 | 1.52632300  | 2.15871000  |
| C | 12.28925000 | 0.86478500  | -1.12078600 |
| H | 10.34750000 | 0.68511000  | -2.03870000 |
| C | 12.98689900 | 1.09798200  | 0.06292800  |
| H | 12.82705200 | 1.51562100  | 2.16812700  |
| H | 12.82930500 | 0.68119800  | -2.04262300 |
| H | 14.07082200 | 1.09481700  | 0.06413800  |
| C | 4.81163800  | 4.00762900  | 0.06222400  |
| H | 4.10839900  | 3.18228800  | 0.08559200  |
| C | 4.34823200  | 5.30012300  | 0.04752900  |
| H | 5.07918700  | 6.10652400  | 0.02961000  |
| C | 2.97757600  | 5.71935300  | 0.05487100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.67681200  | 7.10184500  | 0.04812400  |
| C | 1.87778800  | 4.82634900  | 0.06748500  |
| C | 1.38084100  | 7.56954900  | 0.05475200  |
| H | 3.49799000  | 7.81190100  | 0.03666700  |
| C | 0.57933500  | 5.28122900  | 0.07363600  |
| H | 2.05136800  | 3.75621800  | 0.06961300  |
| C | 0.29513500  | 6.66737400  | 0.06771000  |
| H | 1.18176300  | 8.63581100  | 0.05010500  |
| H | -0.24469100 | 4.57569100  | 0.08268100  |
| N | -0.98928800 | 7.11633200  | 0.09629700  |
| H | -1.18787900 | 8.09666400  | -0.03645600 |
| H | -1.75748200 | 6.47332000  | -0.02384300 |
| C | 4.79447800  | -1.76258900 | 0.04141800  |
| H | 4.09702400  | -0.93300900 | 0.00147800  |
| C | 4.32185400  | -3.05149400 | 0.07167200  |
| H | 5.04652500  | -3.86251300 | 0.11645200  |
| C | 2.94825600  | -3.46054800 | 0.05199100  |
| C | 2.63558300  | -4.83956100 | 0.10127000  |
| C | 1.85666000  | -2.56004600 | -0.01695800 |
| C | 1.33601500  | -5.29698900 | 0.08546600  |
| H | 3.45031100  | -5.55526900 | 0.15264200  |
| C | 0.55481400  | -3.00464600 | -0.03419600 |
| H | 2.03944400  | -1.49233100 | -0.06022400 |
| C | 0.25859100  | -4.38735100 | 0.01681800  |
| H | 1.12769500  | -6.36072100 | 0.12543100  |
| H | -0.26274400 | -2.29364300 | -0.08820900 |
| N | -1.02997400 | -4.82486800 | 0.02180300  |
| H | -1.78802500 | -4.18261700 | -0.15391300 |
| H | -1.23299700 | -5.80904400 | -0.06912900 |