

Optimized Nanotube Dimers

[P-(CH<sub>2</sub>)<sub>7</sub>-P]<sub>4</sub> Dimer

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.03681200  | 0.79610200  | 22.57796800 |
| O | 3.54761400  | -0.32366700 | 22.62088400 |
| C | -0.79610200 | 3.03681200  | 22.57796800 |
| O | 0.32366700  | 3.54761400  | 22.62088400 |
| C | -3.03681200 | -0.79610200 | 22.57796800 |
| O | -3.54761400 | 0.32366700  | 22.62088400 |
| C | 0.79610200  | -3.03681200 | 22.57796800 |
| O | -0.32366700 | -3.54761400 | 22.62088400 |
| H | -2.53763100 | 2.52406300  | 23.53787100 |
| H | 2.52406300  | 2.53763100  | 23.53787100 |
| H | -2.52406300 | -2.53763100 | 23.53787100 |
| H | 2.53763100  | -2.52406300 | 23.53787100 |
| C | -1.30513200 | 2.27200500  | 21.36075900 |
| H | -0.94671900 | 1.23635800  | 21.47289800 |
| H | -2.39333900 | 2.21081300  | 21.34660400 |
| C | 2.27200500  | 1.30513200  | 21.36075900 |
| H | 1.23635800  | 0.94671900  | 21.47289800 |
| H | 2.21081300  | 2.39333900  | 21.34660400 |
| C | -2.27200500 | -1.30513200 | 21.36075900 |
| H | -1.23635800 | -0.94671900 | 21.47289800 |
| H | -2.21081300 | -2.39333900 | 21.34660400 |
| C | 1.30513200  | -2.27200500 | 21.36075900 |
| H | 0.94671900  | -1.23635800 | 21.47289800 |
| H | 2.39333900  | -2.21081300 | 21.34660400 |
| C | 2.66742300  | 1.61721400  | 18.98788300 |
| O | 2.03996800  | 2.68328100  | 19.00625500 |
| C | -1.61721400 | 2.66742300  | 18.98788300 |
| O | -2.68328100 | 2.03996800  | 19.00625500 |
| C | -2.66742300 | -1.61721400 | 18.98788300 |
| O | -2.03996800 | -2.68328100 | 19.00625500 |
| C | 1.61721400  | -2.66742300 | 18.98788300 |
| O | 2.68328100  | -2.03996800 | 19.00625500 |
| C | -1.08375000 | 3.34723000  | 17.73318000 |
| H | 0.00952100  | 3.40362600  | 17.78333600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.45194900 | 4.38401300  | 17.75324000 |
| C | 3.34723000  | 1.08375000  | 17.73318000 |
| H | 3.40362600  | -0.00952100 | 17.78333600 |
| H | 4.38401300  | 1.45194900  | 17.75324000 |
| C | -3.34723000 | -1.08375000 | 17.73318000 |
| H | -3.40362600 | 0.00952100  | 17.78333600 |
| H | -4.38401300 | -1.45194900 | 17.75324000 |
| C | 1.08375000  | -3.34723000 | 17.73318000 |
| H | -0.00952100 | -3.40362600 | 17.78333600 |
| H | 1.45194900  | -4.38401300 | 17.75324000 |
| N | 2.84984400  | 0.86691300  | 20.11178900 |
| N | -0.86691300 | 2.84984400  | 20.11178900 |
| N | -2.84984400 | -0.86691300 | 20.11178900 |
| N | 0.86691300  | -2.84984400 | 20.11178900 |
| H | 3.13927000  | -0.10416500 | 20.01799200 |
| H | 0.10416500  | 3.13927000  | 20.01799200 |
| H | -3.13927000 | 0.10416500  | 20.01799200 |
| H | -0.10416500 | -3.13927000 | 20.01799200 |
| N | -1.67180800 | 3.04652300  | 23.62147300 |
| N | 3.04652300  | 1.67180800  | 23.62147300 |
| N | -3.04652300 | -1.67180800 | 23.62147300 |
| N | 1.67180800  | -3.04652300 | 23.62147300 |
| C | 3.59102100  | 1.32087400  | 24.92144100 |
| H | 4.43518800  | 1.97613500  | 25.17823400 |
| H | 3.95424300  | 0.29494100  | 24.86638100 |
| C | -1.32087400 | 3.59102100  | 24.92144100 |
| H | -1.97613500 | 4.43518800  | 25.17823400 |
| H | -0.29494100 | 3.95424300  | 24.86638100 |
| C | -3.59102100 | -1.32087400 | 24.92144100 |
| H | -4.43518800 | -1.97613500 | 25.17823400 |
| H | -3.95424300 | -0.29494100 | 24.86638100 |
| C | 1.32087400  | -3.59102100 | 24.92144100 |
| H | 0.29494100  | -3.95424300 | 24.86638100 |
| H | 1.97613500  | -4.43518800 | 25.17823400 |
| C | -1.44184600 | 2.54800800  | 26.02521500 |
| O | -0.59877200 | 2.35347100  | 26.88945800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.54800800  | 1.44184600  | 26.02521500 |
| O | 2.35347100  | 0.59877200  | 26.88945800 |
| C | -2.54800800 | -1.44184600 | 26.02521500 |
| O | -2.35347100 | -0.59877200 | 26.88945800 |
| C | 1.44184600  | -2.54800800 | 26.02521500 |
| O | 0.59877200  | -2.35347100 | 26.88945800 |
| O | -2.58551300 | 1.88026800  | 25.94946500 |
| H | -2.55876300 | 1.07167200  | 26.53686400 |
| O | 1.88026800  | 2.58551300  | 25.94946500 |
| H | 1.07167200  | 2.55876300  | 26.53686400 |
| O | -1.88026800 | -2.58551300 | 25.94946500 |
| H | -1.07167200 | -2.55876300 | 26.53686400 |
| O | 2.58551300  | -1.88026800 | 25.94946500 |
| H | 2.55876300  | -1.07167200 | 26.53686400 |
| C | -2.66287800 | -1.54341300 | 16.44229000 |
| H | -2.56154200 | -2.63471100 | 16.46426000 |
| H | -1.63998600 | -1.14138100 | 16.41512400 |
| C | -1.54341300 | 2.66287800  | 16.44229000 |
| H | -1.14138100 | 1.63998600  | 16.41512400 |
| H | -2.63471100 | 2.56154200  | 16.46426000 |
| C | 2.66287800  | 1.54341300  | 16.44229000 |
| H | 1.63998600  | 1.14138100  | 16.41512400 |
| H | 2.56154200  | 2.63471100  | 16.46426000 |
| C | 1.54341300  | -2.66287800 | 16.44229000 |
| H | 2.63471100  | -2.56154200 | 16.46426000 |
| H | 1.14138100  | -1.63998600 | 16.41512400 |
| C | -3.41090700 | -1.11067600 | 15.17534000 |
| H | -4.42898500 | -1.52763500 | 15.19051700 |
| H | -3.52908800 | -0.01744100 | 15.17264800 |
| C | -1.11067600 | 3.41090700  | 15.17534000 |
| H | -1.52763500 | 4.42898500  | 15.19051700 |
| H | -0.01744100 | 3.52908800  | 15.17264800 |
| C | 3.41090700  | 1.11067600  | 15.17534000 |
| H | 4.42898500  | 1.52763500  | 15.19051700 |
| H | 3.52908800  | 0.01744100  | 15.17264800 |
| C | 1.11067600  | -3.41090700 | 15.17534000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.52763500  | -4.42898500 | 15.19051700 |
| H | 0.01744100  | -3.52908800 | 15.17264800 |
| C | -1.54699100 | 2.69900600  | 13.88843700 |
| H | -1.13839100 | 1.67714400  | 13.88900700 |
| H | -2.64150100 | 2.58730600  | 13.88898900 |
| C | 3.04269300  | 0.74484200  | 5.21606900  |
| O | 3.57116700  | -0.36837400 | 5.21013600  |
| C | -0.74484200 | 3.04269300  | 5.21606900  |
| O | 0.36837400  | 3.57116700  | 5.21013600  |
| C | -3.04269300 | -0.74484200 | 5.21606900  |
| O | -3.57116700 | 0.36837400  | 5.21013600  |
| C | 0.74484200  | -3.04269300 | 5.21606900  |
| O | -0.36837400 | -3.57116700 | 5.21013600  |
| H | -2.45969300 | 2.56951600  | 4.17435100  |
| H | 2.56951600  | 2.45969300  | 4.17435100  |
| H | -2.56951600 | -2.45969300 | 4.17435100  |
| H | 2.45969300  | -2.56951600 | 4.17435100  |
| C | -1.28112000 | 2.26734900  | 6.41339100  |
| H | -0.93120300 | 1.22946000  | 6.29940300  |
| H | -2.37020500 | 2.21624600  | 6.41080800  |
| C | 2.26734900  | 1.28112000  | 6.41339100  |
| H | 1.22946000  | 0.93120300  | 6.29940300  |
| H | 2.21624600  | 2.37020500  | 6.41080800  |
| C | -2.26734900 | -1.28112000 | 6.41339100  |
| H | -1.22946000 | -0.93120300 | 6.29940300  |
| H | -2.21624600 | -2.37020500 | 6.41080800  |
| C | 1.28112000  | -2.26734900 | 6.41339100  |
| H | 0.93120300  | -1.22946000 | 6.29940300  |
| H | 2.37020500  | -2.21624600 | 6.41080800  |
| C | 2.66157800  | 1.61201200  | 8.78729000  |
| O | 2.04169500  | 2.68259600  | 8.76360400  |
| C | -1.61201200 | 2.66157800  | 8.78729000  |
| O | -2.68259600 | 2.04169500  | 8.76360400  |
| C | -2.66157800 | -1.61201200 | 8.78729000  |
| O | -2.04169500 | -2.68259600 | 8.76360400  |
| C | 1.61201200  | -2.66157800 | 8.78729000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.68259600  | -2.04169500 | 8.76360400  |
| C | -1.08331200 | 3.34317700  | 10.04327300 |
| H | 0.00982700  | 3.40326000  | 9.99552800  |
| H | -1.45504100 | 4.37868300  | 10.02201500 |
| C | 3.34317700  | 1.08331200  | 10.04327300 |
| H | 3.40326000  | -0.00982700 | 9.99552800  |
| H | 4.37868300  | 1.45504100  | 10.02201500 |
| C | -3.34317700 | -1.08331200 | 10.04327300 |
| H | -3.40326000 | 0.00982700  | 9.99552800  |
| H | -4.37868300 | -1.45504100 | 10.02201500 |
| C | 1.08331200  | -3.34317700 | 10.04327300 |
| H | -0.00982700 | -3.40326000 | 9.99552800  |
| H | 1.45504100  | -4.37868300 | 10.02201500 |
| N | 2.83482200  | 0.85121100  | 7.67023200  |
| N | -0.85121100 | 2.83482200  | 7.67023200  |
| N | -2.83482200 | -0.85121100 | 7.67023200  |
| N | 0.85121100  | -2.83482200 | 7.67023200  |
| H | 3.12548200  | -0.11933000 | 7.76936500  |
| H | 0.11933000  | 3.12548200  | 7.76936500  |
| H | -3.12548200 | 0.11933000  | 7.76936500  |
| H | -0.11933000 | -3.12548200 | 7.76936500  |
| N | -1.56999500 | 3.05366800  | 4.13521700  |
| N | 3.05366800  | 1.56999500  | 4.13521700  |
| N | -3.05366800 | -1.56999500 | 4.13521700  |
| N | 1.56999500  | -3.05366800 | 4.13521700  |
| C | 3.71739300  | 1.16852500  | 2.91368600  |
| H | 4.78887300  | 1.41504700  | 2.93143400  |
| H | 3.66070200  | 0.07960000  | 2.82311100  |
| C | -1.16852500 | 3.71739300  | 2.91368600  |
| H | -1.41504700 | 4.78887300  | 2.93143400  |
| H | -0.07960000 | 3.66070200  | 2.82311100  |
| C | -3.71739300 | -1.16852500 | 2.91368600  |
| H | -4.78887300 | -1.41504700 | 2.93143400  |
| H | -3.66070200 | -0.07960000 | 2.82311100  |
| C | 1.16852500  | -3.71739300 | 2.91368600  |
| H | 0.07960000  | -3.66070200 | 2.82311100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.41504700  | -4.78887300 | 2.93143400  |
| C | -1.77945600 | 3.15618500  | 1.64910400  |
| O | -1.46113300 | 3.61948000  | 0.55755800  |
| C | 3.15618500  | 1.77945600  | 1.64910400  |
| O | 3.61948000  | 1.46113300  | 0.55755800  |
| C | -3.15618500 | -1.77945600 | 1.64910400  |
| O | -3.61948000 | -1.46113300 | 0.55755800  |
| C | 1.77945600  | -3.15618500 | 1.64910400  |
| O | 1.46113300  | -3.61948000 | 0.55755800  |
| O | -2.66169500 | 2.18692900  | 1.82328300  |
| H | -3.04177200 | 1.91582100  | 0.92971700  |
| O | 2.18692900  | 2.66169500  | 1.82328300  |
| H | 1.91582100  | 3.04177200  | 0.92971700  |
| O | -2.18692900 | -2.66169500 | 1.82328300  |
| H | -1.91582100 | -3.04177200 | 0.92971700  |
| O | 2.66169500  | -2.18692900 | 1.82328300  |
| H | 3.04177200  | -1.91582100 | 0.92971700  |
| C | -2.65886900 | -1.54309500 | 11.33410800 |
| H | -2.55602100 | -2.63426100 | 11.31146400 |
| H | -1.63664500 | -1.13941300 | 11.36259100 |
| C | -1.54309500 | 2.65886900  | 11.33410800 |
| H | -1.13941300 | 1.63664500  | 11.36259100 |
| H | -2.63426100 | 2.55602100  | 11.31146400 |
| C | 2.65886900  | 1.54309500  | 11.33410800 |
| H | 1.63664500  | 1.13941300  | 11.36259100 |
| H | 2.55602100  | 2.63426100  | 11.31146400 |
| C | 1.54309500  | -2.65886900 | 11.33410800 |
| H | 2.63426100  | -2.55602100 | 11.31146400 |
| H | 1.13941300  | -1.63664500 | 11.36259100 |
| C | -3.40915200 | -1.11175900 | 12.60028100 |
| H | -4.42669600 | -1.52996400 | 12.58346300 |
| H | -3.52876000 | -0.01867300 | 12.60275500 |
| C | -1.11175900 | 3.40915200  | 12.60028100 |
| H | -1.52996400 | 4.42669600  | 12.58346300 |
| H | -0.01867300 | 3.52876000  | 12.60275500 |
| C | 3.40915200  | 1.11175900  | 12.60028100 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 4.42669600  | 1.52996400  | 12.58346300  |
| H | 3.52876000  | 0.01867300  | 12.60275500  |
| C | 1.11175900  | -3.40915200 | 12.60028100  |
| H | 1.52996400  | -4.42669600 | 12.58346300  |
| H | 0.01867300  | -3.52876000 | 12.60275500  |
| C | 1.54699100  | -2.69900600 | 13.88843700  |
| C | -2.69900600 | -1.54699100 | 13.88843700  |
| C | 2.69900600  | 1.54699100  | 13.88843700  |
| H | 1.67714400  | 1.13839100  | 13.88900700  |
| H | 2.58730600  | 2.64150100  | 13.88898900  |
| H | -1.67714400 | -1.13839100 | 13.88900700  |
| H | -2.58730600 | -2.64150100 | 13.88898900  |
| H | 2.64150100  | -2.58730600 | 13.88898900  |
| H | 1.13839100  | -1.67714400 | 13.88900700  |
| C | -0.79610200 | -3.03681200 | -22.57796800 |
| O | 0.32366700  | -3.54761400 | -22.62088400 |
| C | -3.03681200 | 0.79610200  | -22.57796800 |
| O | -3.54761400 | -0.32366700 | -22.62088400 |
| C | 0.79610200  | 3.03681200  | -22.57796800 |
| O | -0.32366700 | 3.54761400  | -22.62088400 |
| C | 3.03681200  | -0.79610200 | -22.57796800 |
| O | 3.54761400  | 0.32366700  | -22.62088400 |
| H | -2.52406300 | 2.53763100  | -23.53787100 |
| H | -2.53763100 | -2.52406300 | -23.53787100 |
| H | 2.53763100  | 2.52406300  | -23.53787100 |
| H | 2.52406300  | -2.53763100 | -23.53787100 |
| C | -2.27200500 | 1.30513200  | -21.36075900 |
| H | -1.23635800 | 0.94671900  | -21.47289800 |
| H | -2.21081300 | 2.39333900  | -21.34660400 |
| C | -1.30513200 | -2.27200500 | -21.36075900 |
| H | -0.94671900 | -1.23635800 | -21.47289800 |
| H | -2.39333900 | -2.21081300 | -21.34660400 |
| C | 1.30513200  | 2.27200500  | -21.36075900 |
| H | 0.94671900  | 1.23635800  | -21.47289800 |
| H | 2.39333900  | 2.21081300  | -21.34660400 |
| C | 2.27200500  | -1.30513200 | -21.36075900 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 1.23635800  | -0.94671900 | -21.47289800 |
| H | 2.21081300  | -2.39333900 | -21.34660400 |
| C | -1.61721400 | -2.66742300 | -18.98788300 |
| O | -2.68328100 | -2.03996800 | -19.00625500 |
| C | -2.66742300 | 1.61721400  | -18.98788300 |
| O | -2.03996800 | 2.68328100  | -19.00625500 |
| C | 1.61721400  | 2.66742300  | -18.98788300 |
| O | 2.68328100  | 2.03996800  | -19.00625500 |
| C | 2.66742300  | -1.61721400 | -18.98788300 |
| O | 2.03996800  | -2.68328100 | -19.00625500 |
| C | -3.34723000 | 1.08375000  | -17.73318000 |
| H | -3.40362600 | -0.00952100 | -17.78333600 |
| H | -4.38401300 | 1.45194900  | -17.75324000 |
| C | -1.08375000 | -3.34723000 | -17.73318000 |
| H | 0.00952100  | -3.40362600 | -17.78333600 |
| H | -1.45194900 | -4.38401300 | -17.75324000 |
| C | 1.08375000  | 3.34723000  | -17.73318000 |
| H | -0.00952100 | 3.40362600  | -17.78333600 |
| H | 1.45194900  | 4.38401300  | -17.75324000 |
| C | 3.34723000  | -1.08375000 | -17.73318000 |
| H | 3.40362600  | 0.00952100  | -17.78333600 |
| H | 4.38401300  | -1.45194900 | -17.75324000 |
| N | -0.86691300 | -2.84984400 | -20.11178900 |
| N | -2.84984400 | 0.86691300  | -20.11178900 |
| N | 0.86691300  | 2.84984400  | -20.11178900 |
| N | 2.84984400  | -0.86691300 | -20.11178900 |
| H | 0.10416500  | -3.13927000 | -20.01799200 |
| H | -3.13927000 | -0.10416500 | -20.01799200 |
| H | -0.10416500 | 3.13927000  | -20.01799200 |
| H | 3.13927000  | 0.10416500  | -20.01799200 |
| N | -3.04652300 | 1.67180800  | -23.62147300 |
| N | -1.67180800 | -3.04652300 | -23.62147300 |
| N | 1.67180800  | 3.04652300  | -23.62147300 |
| N | 3.04652300  | -1.67180800 | -23.62147300 |
| C | -1.32087400 | -3.59102100 | -24.92144100 |
| H | -1.97613500 | -4.43518800 | -25.17823400 |



|   |             |             |              |
|---|-------------|-------------|--------------|
| H | -0.29494100 | -3.95424300 | -24.86638100 |
| C | -3.59102100 | 1.32087400  | -24.92144100 |
| H | -4.43518800 | 1.97613500  | -25.17823400 |
| H | -3.95424300 | 0.29494100  | -24.86638100 |
| C | 1.32087400  | 3.59102100  | -24.92144100 |
| H | 1.97613500  | 4.43518800  | -25.17823400 |
| H | 0.29494100  | 3.95424300  | -24.86638100 |
| C | 3.59102100  | -1.32087400 | -24.92144100 |
| H | 3.95424300  | -0.29494100 | -24.86638100 |
| H | 4.43518800  | -1.97613500 | -25.17823400 |
| C | -2.54800800 | 1.44184600  | -26.02521500 |
| O | -2.35347100 | 0.59877200  | -26.88945800 |
| C | -1.44184600 | -2.54800800 | -26.02521500 |
| O | -0.59877200 | -2.35347100 | -26.88945800 |
| C | 1.44184600  | 2.54800800  | -26.02521500 |
| O | 0.59877200  | 2.35347100  | -26.88945800 |
| C | 2.54800800  | -1.44184600 | -26.02521500 |
| O | 2.35347100  | -0.59877200 | -26.88945800 |
| O | -1.88026800 | 2.58551300  | -25.94946500 |
| H | -1.07167200 | 2.55876300  | -26.53686400 |
| O | -2.58551300 | -1.88026800 | -25.94946500 |
| H | -2.55876300 | -1.07167200 | -26.53686400 |
| O | 2.58551300  | 1.88026800  | -25.94946500 |
| H | 2.55876300  | 1.07167200  | -26.53686400 |
| O | 1.88026800  | -2.58551300 | -25.94946500 |
| H | 1.07167200  | -2.55876300 | -26.53686400 |
| C | 1.54341300  | 2.66287800  | -16.44229000 |
| H | 2.63471100  | 2.56154200  | -16.46426000 |
| H | 1.14138100  | 1.63998600  | -16.41512400 |
| C | -2.66287800 | 1.54341300  | -16.44229000 |
| H | -1.63998600 | 1.14138100  | -16.41512400 |
| H | -2.56154200 | 2.63471100  | -16.46426000 |
| C | -1.54341300 | -2.66287800 | -16.44229000 |
| H | -1.14138100 | -1.63998600 | -16.41512400 |
| H | -2.63471100 | -2.56154200 | -16.46426000 |
| C | 2.66287800  | -1.54341300 | -16.44229000 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 2.56154200  | -2.63471100 | -16.46426000 |
| H | 1.63998600  | -1.14138100 | -16.41512400 |
| C | 1.11067600  | 3.41090700  | -15.17534000 |
| H | 1.52763500  | 4.42898500  | -15.19051700 |
| H | 0.01744100  | 3.52908800  | -15.17264800 |
| C | -3.41090700 | 1.11067600  | -15.17534000 |
| H | -4.42898500 | 1.52763500  | -15.19051700 |
| H | -3.52908800 | 0.01744100  | -15.17264800 |
| C | -1.11067600 | -3.41090700 | -15.17534000 |
| H | -1.52763500 | -4.42898500 | -15.19051700 |
| H | -0.01744100 | -3.52908800 | -15.17264800 |
| C | 3.41090700  | -1.11067600 | -15.17534000 |
| H | 4.42898500  | -1.52763500 | -15.19051700 |
| H | 3.52908800  | -0.01744100 | -15.17264800 |
| C | -2.69900600 | 1.54699100  | -13.88843700 |
| H | -1.67714400 | 1.13839100  | -13.88900700 |
| H | -2.58730600 | 2.64150100  | -13.88898900 |
| C | -0.74484200 | -3.04269300 | -5.21606900  |
| O | 0.36837400  | -3.57116700 | -5.21013600  |
| C | -3.04269300 | 0.74484200  | -5.21606900  |
| O | -3.57116700 | -0.36837400 | -5.21013600  |
| C | 0.74484200  | 3.04269300  | -5.21606900  |
| O | -0.36837400 | 3.57116700  | -5.21013600  |
| C | 3.04269300  | -0.74484200 | -5.21606900  |
| O | 3.57116700  | 0.36837400  | -5.21013600  |
| H | -2.56951600 | 2.45969300  | -4.17435100  |
| H | -2.45969300 | -2.56951600 | -4.17435100  |
| H | 2.45969300  | 2.56951600  | -4.17435100  |
| H | 2.56951600  | -2.45969300 | -4.17435100  |
| C | -2.26734900 | 1.28112000  | -6.41339100  |
| H | -1.22946000 | 0.93120300  | -6.29940300  |
| H | -2.21624600 | 2.37020500  | -6.41080800  |
| C | -1.28112000 | -2.26734900 | -6.41339100  |
| H | -0.93120300 | -1.22946000 | -6.29940300  |
| H | -2.37020500 | -2.21624600 | -6.41080800  |
| C | 1.28112000  | 2.26734900  | -6.41339100  |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 0.93120300  | 1.22946000  | -6.29940300  |
| H | 2.37020500  | 2.21624600  | -6.41080800  |
| C | 2.26734900  | -1.28112000 | -6.41339100  |
| H | 1.22946000  | -0.93120300 | -6.29940300  |
| H | 2.21624600  | -2.37020500 | -6.41080800  |
| C | -1.61201200 | -2.66157800 | -8.78729000  |
| O | -2.68259600 | -2.04169500 | -8.76360400  |
| C | -2.66157800 | 1.61201200  | -8.78729000  |
| O | -2.04169500 | 2.68259600  | -8.76360400  |
| C | 1.61201200  | 2.66157800  | -8.78729000  |
| O | 2.68259600  | 2.04169500  | -8.76360400  |
| C | 2.66157800  | -1.61201200 | -8.78729000  |
| O | 2.04169500  | -2.68259600 | -8.76360400  |
| C | -3.34317700 | 1.08331200  | -10.04327300 |
| H | -3.40326000 | -0.00982700 | -9.99552800  |
| H | -4.37868300 | 1.45504100  | -10.02201500 |
| C | -1.08331200 | -3.34317700 | -10.04327300 |
| H | 0.00982700  | -3.40326000 | -9.99552800  |
| H | -1.45504100 | -4.37868300 | -10.02201500 |
| C | 1.08331200  | 3.34317700  | -10.04327300 |
| H | -0.00982700 | 3.40326000  | -9.99552800  |
| H | 1.45504100  | 4.37868300  | -10.02201500 |
| C | 3.34317700  | -1.08331200 | -10.04327300 |
| H | 3.40326000  | 0.00982700  | -9.99552800  |
| H | 4.37868300  | -1.45504100 | -10.02201500 |
| N | -0.85121100 | -2.83482200 | -7.67023200  |
| N | -2.83482200 | 0.85121100  | -7.67023200  |
| N | 0.85121100  | 2.83482200  | -7.67023200  |
| N | 2.83482200  | -0.85121100 | -7.67023200  |
| H | 0.11933000  | -3.12548200 | -7.76936500  |
| H | -3.12548200 | -0.11933000 | -7.76936500  |
| H | -0.11933000 | 3.12548200  | -7.76936500  |
| H | 3.12548200  | 0.11933000  | -7.76936500  |
| N | -3.05366800 | 1.56999500  | -4.13521700  |
| N | -1.56999500 | -3.05366800 | -4.13521700  |
| N | 1.56999500  | 3.05366800  | -4.13521700  |

|   |             |             |              |
|---|-------------|-------------|--------------|
| N | 3.05366800  | -1.56999500 | -4.13521700  |
| C | -1.16852500 | -3.71739300 | -2.91368600  |
| H | -1.41504700 | -4.78887300 | -2.93143400  |
| H | -0.07960000 | -3.66070200 | -2.82311100  |
| C | -3.71739300 | 1.16852500  | -2.91368600  |
| H | -4.78887300 | 1.41504700  | -2.93143400  |
| H | -3.66070200 | 0.07960000  | -2.82311100  |
| C | 1.16852500  | 3.71739300  | -2.91368600  |
| H | 1.41504700  | 4.78887300  | -2.93143400  |
| H | 0.07960000  | 3.66070200  | -2.82311100  |
| C | 3.71739300  | -1.16852500 | -2.91368600  |
| H | 3.66070200  | -0.07960000 | -2.82311100  |
| H | 4.78887300  | -1.41504700 | -2.93143400  |
| C | -3.15618500 | 1.77945600  | -1.64910400  |
| O | -3.61948000 | 1.46113300  | -0.55755800  |
| C | -1.77945600 | -3.15618500 | -1.64910400  |
| O | -1.46113300 | -3.61948000 | -0.55755800  |
| C | 1.77945600  | 3.15618500  | -1.64910400  |
| O | 1.46113300  | 3.61948000  | -0.55755800  |
| C | 3.15618500  | -1.77945600 | -1.64910400  |
| O | 3.61948000  | -1.46113300 | -0.55755800  |
| O | -2.18692900 | 2.66169500  | -1.82328300  |
| H | -1.91582100 | 3.04177200  | -0.92971700  |
| O | -2.66169500 | -2.18692900 | -1.82328300  |
| H | -3.04177200 | -1.91582100 | -0.92971700  |
| O | 2.66169500  | 2.18692900  | -1.82328300  |
| H | 3.04177200  | 1.91582100  | -0.92971700  |
| O | 2.18692900  | -2.66169500 | -1.82328300  |
| H | 1.91582100  | -3.04177200 | -0.92971700  |
| C | 1.54309500  | 2.65886900  | -11.33410800 |
| H | 2.63426100  | 2.55602100  | -11.31146400 |
| H | 1.13941300  | 1.63664500  | -11.36259100 |
| C | -2.65886900 | 1.54309500  | -11.33410800 |
| H | -1.63664500 | 1.13941300  | -11.36259100 |
| H | -2.55602100 | 2.63426100  | -11.31146400 |
| C | -1.54309500 | -2.65886900 | -11.33410800 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | -1.13941300 | -1.63664500 | -11.36259100 |
| H | -2.63426100 | -2.55602100 | -11.31146400 |
| C | 2.65886900  | -1.54309500 | -11.33410800 |
| H | 2.55602100  | -2.63426100 | -11.31146400 |
| H | 1.63664500  | -1.13941300 | -11.36259100 |
| C | 1.11175900  | 3.40915200  | -12.60028100 |
| H | 1.52996400  | 4.42669600  | -12.58346300 |
| H | 0.01867300  | 3.52876000  | -12.60275500 |
| C | -3.40915200 | 1.11175900  | -12.60028100 |
| H | -4.42669600 | 1.52996400  | -12.58346300 |
| H | -3.52876000 | 0.01867300  | -12.60275500 |
| C | -1.11175900 | -3.40915200 | -12.60028100 |
| H | -1.52996400 | -4.42669600 | -12.58346300 |
| H | -0.01867300 | -3.52876000 | -12.60275500 |
| C | 3.40915200  | -1.11175900 | -12.60028100 |
| H | 4.42669600  | -1.52996400 | -12.58346300 |
| H | 3.52876000  | -0.01867300 | -12.60275500 |
| C | 2.69900600  | -1.54699100 | -13.88843700 |
| C | 1.54699100  | 2.69900600  | -13.88843700 |
| C | -1.54699100 | -2.69900600 | -13.88843700 |
| H | -1.13839100 | -1.67714400 | -13.88900700 |
| H | -2.64150100 | -2.58730600 | -13.88898900 |
| H | 1.13839100  | 1.67714400  | -13.88900700 |
| H | 2.64150100  | 2.58730600  | -13.88898900 |
| H | 2.58730600  | -2.64150100 | -13.88898900 |
| H | 1.67714400  | -1.13839100 | -13.88900700 |

### [P-(CH<sub>2</sub>)<sub>7</sub>-P]<sub>6</sub> Dimer

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -0.69353500 | -4.40633500 | 5.19690000 |
| O | 0.44987900  | -4.87071400 | 5.11684100 |
| C | 3.46923100  | -2.80378600 | 5.19690000 |
| O | 4.44310200  | -2.04575000 | 5.11684100 |
| C | 4.16276500  | 1.60254900  | 5.19690000 |
| O | 3.99322300  | 2.82496400  | 5.11684100 |
| C | -3.46923100 | 2.80378600  | 5.19690000 |
| O | -4.44310200 | 2.04575000  | 5.11684100 |
| C | -4.16276500 | -1.60254900 | 5.19690000 |

|   |             |             |            |
|---|-------------|-------------|------------|
| O | -3.99322300 | -2.82496400 | 5.11684100 |
| C | 0.69353500  | 4.40633500  | 5.19690000 |
| O | -0.44987900 | 4.87071400  | 5.11684100 |
| H | -2.55790600 | -4.16383000 | 4.36424000 |
| H | 2.32702900  | -4.29712600 | 4.36424000 |
| H | 4.88493500  | -0.13329600 | 4.36424000 |
| H | -2.32702900 | 4.29712600  | 4.36424000 |
| H | -4.88493500 | 0.13329600  | 4.36424000 |
| H | 2.55790600  | 4.16383000  | 4.36424000 |
| C | -1.13754900 | -3.57740700 | 6.40191500 |
| H | -2.21704000 | -3.43686300 | 6.39387600 |
| H | -0.66405000 | -2.58709400 | 6.30785600 |
| C | 2.52935100  | -2.77384900 | 6.40191500 |
| H | 1.86789100  | -3.63844400 | 6.39387600 |
| H | 1.90846400  | -1.86863100 | 6.30785600 |
| C | 3.66689900  | 0.80355700  | 6.40191500 |
| H | 4.08493000  | -0.20158100 | 6.39387600 |
| H | 2.57251400  | 0.71846200  | 6.30785600 |
| C | -2.52935100 | 2.77384900  | 6.40191500 |
| H | -1.86789100 | 3.63844400  | 6.39387600 |
| H | -1.90846400 | 1.86863100  | 6.30785600 |
| C | -3.66689900 | -0.80355700 | 6.40191500 |
| H | -4.08493000 | 0.20158100  | 6.39387600 |
| H | -2.57251400 | -0.71846200 | 6.30785600 |
| C | 1.13754900  | 3.57740700  | 6.40191500 |
| H | 2.21704000  | 3.43686300  | 6.39387600 |
| H | 0.66405000  | 2.58709400  | 6.30785600 |
| C | -1.66096600 | -4.34241600 | 8.66814900 |
| O | -2.83391800 | -3.94783200 | 8.59708900 |
| C | 2.93015900  | -3.60964600 | 8.66814900 |
| O | 2.00196400  | -4.42816000 | 8.59708900 |
| C | 4.59112500  | 0.73276900  | 8.66814900 |
| O | 4.83588100  | -0.48032900 | 8.59708900 |
| C | -2.93015900 | 3.60964600  | 8.66814900 |
| O | -2.00196400 | 4.42816000  | 8.59708900 |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -4.59112500 | -0.73276900 | 8.66814900 |
| O | -4.83588100 | 0.48032900  | 8.59708900 |
| C | 1.66096600  | 4.34241600  | 8.66814900 |
| O | 2.83391800  | 3.94783200  | 8.59708900 |
| C | -1.13392900 | -5.04970100 | 9.90991900 |
| H | -0.04355700 | -5.13675400 | 9.86268000 |
| H | -1.54119700 | -6.07082600 | 9.88865100 |
| C | 3.80620500  | -3.50686200 | 9.90991900 |
| H | 4.42678100  | -2.60609800 | 9.86268000 |
| H | 4.48689100  | -4.37012900 | 9.88865100 |
| C | 4.94013400  | 1.54283900  | 9.90991900 |
| H | 4.47033800  | 2.53065600  | 9.86268000 |
| H | 6.02808800  | 1.70069700  | 9.88865100 |
| C | -3.80620500 | 3.50686200  | 9.90991900 |
| H | -4.42678100 | 2.60609800  | 9.86268000 |
| H | -4.48689100 | 4.37012900  | 9.88865100 |
| C | -4.94013400 | -1.54283900 | 9.90991900 |
| H | -4.47033800 | -2.53065600 | 9.86268000 |
| H | -6.02808800 | -1.70069700 | 9.88865100 |
| C | 1.13392900  | 5.04970100  | 9.90991900 |
| H | 0.04355700  | 5.13675400  | 9.86268000 |
| H | 1.54119700  | 6.07082600  | 9.88865100 |
| N | -0.76975700 | -4.20589500 | 7.65345400 |
| N | 3.25753300  | -2.76957600 | 7.65345400 |
| N | 4.02729000  | 1.43631900  | 7.65345400 |
| N | -3.25753300 | 2.76957600  | 7.65345400 |
| N | -4.02729000 | -1.43631900 | 7.65345400 |
| N | 0.76975700  | 4.20589500  | 7.65345400 |
| H | 3.94511000  | -2.03234400 | 7.82258100 |
| H | 3.73261600  | 2.40039300  | 7.82258100 |
| H | 0.21249400  | -4.43273700 | 7.82258100 |
| H | -3.94511000 | 2.03234400  | 7.82258100 |
| H | -3.73261600 | -2.40039300 | 7.82258100 |
| H | -0.21249400 | 4.43273700  | 7.82258100 |
| N | -1.63185600 | -4.56770000 | 4.23218400 |

|   |             |             |            |
|---|-------------|-------------|------------|
| N | 3.13981600  | -3.69707800 | 4.23218400 |
| N | 4.77167200  | 0.87062100  | 4.23218400 |
| N | -3.13981600 | 3.69707800  | 4.23218400 |
| N | -4.77167200 | -0.87062100 | 4.23218400 |
| N | 1.63185600  | 4.56770000  | 4.23218400 |
| C | 3.98031400  | -3.85517900 | 3.06305700 |
| H | 4.63006400  | -4.73896100 | 3.16284700 |
| H | 4.63346900  | -2.98504700 | 2.99262200 |
| C | -1.34852500 | -5.37464300 | 3.06305700 |
| H | -1.78902800 | -6.37923400 | 3.16284700 |
| H | -0.26839200 | -5.50522500 | 2.99262200 |
| C | -5.32884000 | -1.51946400 | 3.06305700 |
| H | -4.90186100 | -2.52017800 | 2.99262200 |
| H | -6.41909300 | -1.64027300 | 3.16284700 |
| C | -3.98031400 | 3.85517900  | 3.06305700 |
| H | -4.63006400 | 4.73896100  | 3.16284700 |
| H | -4.63346900 | 2.98504700  | 2.99262200 |
| C | 1.34852500  | 5.37464300  | 3.06305700 |
| H | 0.26839200  | 5.50522500  | 2.99262200 |
| H | 1.78902800  | 6.37923400  | 3.16284700 |
| C | 5.32884000  | 1.51946400  | 3.06305700 |
| H | 6.41909300  | 1.64027300  | 3.16284700 |
| H | 4.90186100  | 2.52017800  | 2.99262200 |
| C | 1.85144600  | 4.82495200  | 1.74306700 |
| O | 1.31303900  | 5.16119800  | 0.69330800 |
| C | 3.25280800  | -4.01587500 | 1.74306700 |
| O | 3.81320900  | -3.71772400 | 0.69330800 |
| C | -1.85144600 | -4.82495200 | 1.74306700 |
| O | -1.31303900 | -5.16119800 | 0.69330800 |
| C | -5.10425400 | -0.80907700 | 1.74306700 |
| O | -5.12624800 | -1.44347400 | 0.69330800 |
| C | -3.25280800 | 4.01587500  | 1.74306700 |
| O | -3.81320900 | 3.71772400  | 0.69330800 |
| C | 5.10425400  | 0.80907700  | 1.74306700 |
| O | 5.12624800  | 1.44347400  | 0.69330800 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.91830300  | 4.04814500  | 1.82541700  |
| H | 3.24824600  | 3.84585500  | 0.89814100  |
| O | 2.04664500  | -4.55139600 | 1.82541700  |
| H | 1.70648600  | -4.73599100 | 0.89814100  |
| O | -2.91830300 | -4.04814500 | 1.82541700  |
| H | -3.24824600 | -3.84585500 | 0.89814100  |
| O | -4.96494700 | 0.50325200  | 1.82541700  |
| H | -4.95473100 | 0.89013500  | 0.89814100  |
| O | -2.04664500 | 4.55139600  | 1.82541700  |
| H | -1.70648600 | 4.73599100  | 0.89814100  |
| O | 4.96494700  | -0.50325200 | 1.82541700  |
| H | 4.95473100  | -0.89013500 | 0.89814100  |
| C | -1.57471800 | -4.35447600 | 11.20549500 |
| C | -1.14199700 | -5.10402200 | 12.47135000 |
| H | -1.16004300 | -3.33646000 | 11.22715300 |
| H | -2.66543500 | -4.24483600 | 11.19147600 |
| C | -1.57355500 | -4.39057100 | 13.75904800 |
| H | -0.04892800 | -5.22620500 | 12.47119200 |
| H | -1.56269900 | -6.12044500 | 12.45651400 |
| C | -2.98372800 | 3.54098300  | 11.20549500 |
| C | -3.84921400 | 3.54100900  | 12.47135000 |
| H | -2.30943800 | 2.67285600  | 11.22715300 |
| H | -2.34341800 | 4.43075200  | 11.19147600 |
| C | -3.01556800 | 3.55802400  | 13.75904800 |
| H | -4.50156200 | 2.65547500  | 12.47119200 |
| H | -4.51911100 | 4.41355900  | 12.45651400 |
| C | 2.98372800  | -3.54098300 | 11.20549500 |
| C | 3.84921400  | -3.54100900 | 12.47135000 |
| H | 2.30943800  | -2.67285600 | 11.22715300 |
| H | 2.34341800  | -4.43075200 | 11.19147600 |
| C | 3.01556800  | -3.55802400 | 13.75904800 |
| H | 4.50156200  | -2.65547500 | 12.47119200 |
| H | 4.51911100  | -4.41355900 | 12.45651400 |
| C | 4.55844500  | 0.81349200  | 11.20549500 |
| C | 4.99121100  | 1.56301300  | 12.47135000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.46948000  | 0.66360400  | 11.22715300 |
| H | 5.00885300  | -0.18591600 | 11.19147600 |
| C | 4.58912300  | 0.83254700  | 13.75904800 |
| H | 4.55049000  | 2.57073000  | 12.47119200 |
| H | 6.08181000  | 1.70688500  | 12.45651400 |
| C | -4.55844500 | -0.81349200 | 11.20549500 |
| C | -4.99121100 | -1.56301300 | 12.47135000 |
| H | -3.46948000 | -0.66360400 | 11.22715300 |
| H | -5.00885300 | 0.18591600  | 11.19147600 |
| C | -4.58912300 | -0.83254700 | 13.75904800 |
| H | -4.55049000 | -2.57073000 | 12.47119200 |
| H | -6.08181000 | -1.70688500 | 12.45651400 |
| C | 1.57471800  | 4.35447600  | 11.20549500 |
| C | 1.14199700  | 5.10402200  | 12.47135000 |
| H | 1.16004300  | 3.33646000  | 11.22715300 |
| H | 2.66543500  | 4.24483600  | 11.19147600 |
| C | 1.57355500  | 4.39057100  | 13.75904800 |
| H | 0.04892800  | 5.22620500  | 12.47119200 |
| H | 1.56269900  | 6.12044500  | 12.45651400 |
| C | -0.75999800 | -4.39849700 | 22.36340200 |
| O | 0.37736300  | -4.86898700 | 22.47447500 |
| C | 3.42921100  | -2.85742600 | 22.36340200 |
| O | 4.40534800  | -2.10768700 | 22.47447500 |
| C | 4.18920900  | 1.54107100  | 22.36340200 |
| O | 4.02798500  | 2.76130000  | 22.47447500 |
| C | -3.42921100 | 2.85742600  | 22.36340200 |
| O | -4.40534800 | 2.10768700  | 22.47447500 |
| C | -4.18920900 | -1.54107100 | 22.36340200 |
| O | -4.02798500 | -2.76130000 | 22.47447500 |
| C | 0.75999800  | 4.39849700  | 22.36340200 |
| O | -0.37736300 | 4.86898700  | 22.47447500 |
| H | -2.61381800 | -4.03530500 | 23.16425400 |
| H | 2.18776700  | -4.28128500 | 23.16425400 |
| H | 4.80158500  | -0.24598000 | 23.16425400 |
| H | -2.18776700 | 4.28128500  | 23.16425400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.80158500 | 0.24598000  | 23.16425400 |
| H | 2.61381800  | 4.03530500  | 23.16425400 |
| C | -1.19719900 | -3.62288600 | 21.12015300 |
| H | -2.27775300 | -3.48989400 | 21.11235800 |
| H | -0.73803500 | -2.62326400 | 21.19725700 |
| C | 2.53891200  | -2.84824700 | 21.12015300 |
| H | 1.88346000  | -3.71753800 | 21.11235800 |
| H | 1.90279500  | -1.95078900 | 21.19725700 |
| C | 3.73611000  | 0.77463900  | 21.12015300 |
| H | 4.16121300  | -0.22764500 | 21.11235800 |
| H | 2.64083100  | 0.67247500  | 21.19725700 |
| C | -2.53891200 | 2.84824700  | 21.12015300 |
| H | -1.88346000 | 3.71753800  | 21.11235800 |
| H | -1.90279500 | 1.95078900  | 21.19725700 |
| C | -3.73611000 | -0.77463900 | 21.12015300 |
| H | -4.16121300 | 0.22764500  | 21.11235800 |
| H | -2.64083100 | -0.67247500 | 21.19725700 |
| C | 1.19719900  | 3.62288600  | 21.12015300 |
| H | 2.27775300  | 3.48989400  | 21.11235800 |
| H | 0.73803500  | 2.62326400  | 21.19725700 |
| C | -1.69318100 | -4.36654500 | 18.84972100 |
| O | -2.85532200 | -3.94065100 | 18.90992000 |
| C | 2.93494800  | -3.64961000 | 18.84972100 |
| O | 1.98504300  | -4.44310600 | 18.90992000 |
| C | 4.62812900  | 0.71693500  | 18.84972100 |
| O | 4.84036400  | -0.50245600 | 18.90992000 |
| C | -2.93494800 | 3.64961000  | 18.84972100 |
| O | -1.98504300 | 4.44310600  | 18.90992000 |
| C | -4.62812900 | -0.71693500 | 18.84972100 |
| O | -4.84036400 | 0.50245600  | 18.90992000 |
| C | 1.69318100  | 4.36654500  | 18.84972100 |
| O | 2.85532200  | 3.94065100  | 18.90992000 |
| C | -1.16342200 | -5.07023900 | 17.60750300 |
| H | -0.07357300 | -5.16190000 | 17.66089400 |
| H | -1.57412600 | -6.09018500 | 17.62181600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.80924500  | -3.54267200 | 17.60750300 |
| H | 4.43355000  | -2.64466600 | 17.66089400 |
| H | 4.48719200  | -4.40832500 | 17.62181600 |
| C | 4.97266700  | 1.52756700  | 17.60750300 |
| H | 4.50712300  | 2.51723400  | 17.66089400 |
| H | 6.06131800  | 1.68185900  | 17.62181600 |
| C | -3.80924500 | 3.54267200  | 17.60750300 |
| H | -4.43355000 | 2.64466600  | 17.66089400 |
| H | -4.48719200 | 4.40832500  | 17.62181600 |
| C | -4.97266700 | -1.52756700 | 17.60750300 |
| H | -4.50712300 | -2.51723400 | 17.66089400 |
| H | -6.06131800 | -1.68185900 | 17.62181600 |
| C | 1.16342200  | 5.07023900  | 17.60750300 |
| H | 0.07357300  | 5.16190000  | 17.66089400 |
| H | 1.57412600  | 6.09018500  | 17.62181600 |
| N | -0.81663200 | -4.27005600 | 19.88406500 |
| N | 3.28966100  | -2.84225200 | 19.88406500 |
| N | 4.10629300  | 1.42780400  | 19.88406500 |
| N | -3.28966100 | 2.84225200  | 19.88406500 |
| N | -4.10629300 | -1.42780400 | 19.88406500 |
| N | 0.81663200  | 4.27005600  | 19.88406500 |
| H | 3.97334300  | -2.10142800 | 19.72042000 |
| H | 3.80656100  | 2.39030200  | 19.72042000 |
| H | 0.16678200  | -4.49173000 | 19.72042000 |
| H | -3.97334300 | 2.10142800  | 19.72042000 |
| H | -3.80656100 | -2.39030200 | 19.72042000 |
| H | -0.16678200 | 4.49173000  | 19.72042000 |
| N | -1.70736700 | -4.47336400 | 23.32948300 |
| N | 3.02036300  | -3.71530500 | 23.32948300 |
| N | 4.72773000  | 0.75805900  | 23.32948300 |
| N | -3.02036300 | 3.71530500  | 23.32948300 |
| N | -4.72773000 | -0.75805900 | 23.32948300 |
| N | 1.70736700  | 4.47336400  | 23.32948300 |
| C | 3.64931100  | -3.77341000 | 24.64113300 |
| H | 4.04536900  | -4.77941100 | 24.82896000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.46763900  | -3.05560300 | 24.65766400 |
| C | -1.44321300 | -5.04710100 | 24.64113300 |
| H | -2.11640600 | -5.89309800 | 24.82896000 |
| H | -0.41241000 | -5.39689000 | 24.65766400 |
| C | -5.09252400 | -1.27369200 | 24.64113300 |
| H | -4.88004900 | -2.34128700 | 24.65766400 |
| H | -6.16177600 | -1.11368700 | 24.82896000 |
| C | -3.64931100 | 3.77341000  | 24.64113300 |
| H | -4.04536900 | 4.77941100  | 24.82896000 |
| H | -4.46763900 | 3.05560300  | 24.65766400 |
| C | 1.44321300  | 5.04710100  | 24.64113300 |
| H | 0.41241000  | 5.39689000  | 24.65766400 |
| H | 2.11640600  | 5.89309800  | 24.82896000 |
| C | 5.09252400  | 1.27369200  | 24.64113300 |
| H | 6.16177600  | 1.11368700  | 24.82896000 |
| H | 4.88004900  | 2.34128700  | 24.65766400 |
| C | 1.66813900  | 3.99704900  | 25.72639000 |
| O | 0.81721100  | 3.59449500  | 26.50838600 |
| C | 2.62747600  | -3.44317500 | 25.72639000 |
| O | 2.70431900  | -2.50497300 | 26.50838600 |
| C | -1.66813900 | -3.99704900 | 25.72639000 |
| O | -0.81721100 | -3.59449500 | 26.50838600 |
| C | -4.29561500 | -0.55387400 | 25.72639000 |
| O | -3.52152900 | -1.08952200 | 26.50838600 |
| C | -2.62747600 | 3.44317500  | 25.72639000 |
| O | -2.70431900 | 2.50497300  | 26.50838600 |
| C | 4.29561500  | 0.55387400  | 25.72639000 |
| O | 3.52152900  | 1.08952200  | 26.50838600 |
| O | 2.91586800  | 3.55274200  | 25.70336000 |
| H | 3.03396900  | 2.71653800  | 26.24038500 |
| O | 1.61883100  | -4.30158600 | 25.70336000 |
| H | 0.83560600  | -3.98576300 | 26.24038500 |
| O | -2.91586800 | -3.55274200 | 25.70336000 |
| H | -3.03396900 | -2.71653800 | 26.24038500 |
| O | -4.53469800 | 0.74884500  | 25.70336000 |

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|---|-------------|-------------|-------------|
| H | -3.86957500 | 1.26922600  | 26.24038500 |
| O | -1.61883100 | 4.30158600  | 25.70336000 |
| H | -0.83560600 | 3.98576300  | 26.24038500 |
| O | 4.53469800  | -0.74884500 | 25.70336000 |
| H | 3.86957500  | -1.26922600 | 26.24038500 |
| C | -1.59300600 | -4.36716800 | 16.31262300 |
| C | -1.15232900 | -5.11110600 | 15.04621800 |
| H | -1.17577800 | -3.35010400 | 16.29951500 |
| H | -2.68346600 | -4.25447300 | 16.31910700 |
| H | -0.05945800 | -5.23486700 | 15.05370400 |
| H | -1.57454100 | -6.12699100 | 15.05282300 |
| C | -2.98557500 | 3.56316700  | 16.31262300 |
| C | -3.85018300 | 3.55349900  | 15.04621800 |
| H | -2.31338600 | 2.69330500  | 16.29951500 |
| H | -2.34274800 | 4.45118600  | 16.31910700 |
| H | -4.50379900 | 2.66892500  | 15.05370400 |
| H | -4.51885900 | 4.42708800  | 15.05282300 |
| C | 2.98557500  | -3.56316700 | 16.31262300 |
| C | 3.85018300  | -3.55349900 | 15.04621800 |
| H | 2.31338600  | -2.69330500 | 16.29951500 |
| H | 2.34274800  | -4.45118600 | 16.31910700 |
| H | 4.50379900  | -2.66892500 | 15.05370400 |
| H | 4.51885900  | -4.42708800 | 15.05282300 |
| C | 4.57858100  | 0.80400000  | 16.31262300 |
| C | 5.00251200  | 1.55760700  | 15.04621800 |
| H | 3.48916400  | 0.65679900  | 16.29951500 |
| H | 5.02621400  | -0.19671300 | 16.31910700 |
| H | 4.56325700  | 2.56594100  | 15.05370400 |
| H | 6.09340000  | 1.69990300  | 15.05282300 |
| C | -4.57858100 | -0.80400000 | 16.31262300 |
| C | -5.00251200 | -1.55760700 | 15.04621800 |
| H | -3.48916400 | -0.65679900 | 16.29951500 |
| H | -5.02621400 | 0.19671300  | 16.31910700 |
| H | -4.56325700 | -2.56594100 | 15.05370400 |
| H | -6.09340000 | -1.69990300 | 15.05282300 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| C | 1.59300600  | 4.36716800  | 16.31262300  |
| C | 1.15232900  | 5.11110600  | 15.04621800  |
| H | 1.17577800  | 3.35010400  | 16.29951500  |
| H | 2.68346600  | 4.25447300  | 16.31910700  |
| H | 0.05945800  | 5.23486700  | 15.05370400  |
| H | 1.57454100  | 6.12699100  | 15.05282300  |
| H | 2.36347400  | -4.44425900 | 13.75504000  |
| H | 2.34336300  | -2.68704800 | 13.76350300  |
| H | -1.15537100 | -3.37293600 | 13.76350300  |
| H | -2.66710400 | -4.26895800 | 13.75504000  |
| H | -3.49873300 | -0.68588700 | 13.76350300  |
| H | -5.03057900 | 0.17530100  | 13.75504000  |
| H | -2.34336300 | 2.68704800  | 13.76350300  |
| H | -2.36347400 | 4.44425900  | 13.75504000  |
| H | 2.66710400  | 4.26895800  | 13.75504000  |
| H | 1.15537100  | 3.37293600  | 13.76350300  |
| H | 5.03057900  | -0.17530100 | 13.75504000  |
| H | 3.49873300  | 0.68588700  | 13.76350300  |
| C | 3.42921100  | 2.85742600  | -22.36340200 |
| O | 4.40534800  | 2.10768700  | -22.47447500 |
| C | 4.18920900  | -1.54107100 | -22.36340200 |
| O | 4.02798500  | -2.76130000 | -22.47447500 |
| C | 0.75999800  | -4.39849700 | -22.36340200 |
| O | -0.37736300 | -4.86898700 | -22.47447500 |
| C | -4.18920900 | 1.54107100  | -22.36340200 |
| O | -4.02798500 | 2.76130000  | -22.47447500 |
| C | -0.75999800 | 4.39849700  | -22.36340200 |
| O | 0.37736300  | 4.86898700  | -22.47447500 |
| C | -3.42921100 | -2.85742600 | -22.36340200 |
| O | -4.40534800 | -2.10768700 | -22.47447500 |
| H | 2.18776700  | 4.28128500  | -23.16425400 |
| H | 4.80158500  | 0.24598000  | -23.16425400 |
| H | 2.61381800  | -4.03530500 | -23.16425400 |
| H | -4.80158500 | -0.24598000 | -23.16425400 |
| H | -2.61381800 | 4.03530500  | -23.16425400 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | -2.18776700 | -4.28128500 | -23.16425400 |
| C | 2.53891200  | 2.84824700  | -21.12015300 |
| H | 1.88346000  | 3.71753800  | -21.11235800 |
| H | 1.90279500  | 1.95078900  | -21.19725700 |
| C | 3.73611000  | -0.77463900 | -21.12015300 |
| H | 4.16121300  | 0.22764500  | -21.11235800 |
| H | 2.64083100  | -0.67247500 | -21.19725700 |
| C | 1.19719900  | -3.62288600 | -21.12015300 |
| H | 2.27775300  | -3.48989400 | -21.11235800 |
| H | 0.73803500  | -2.62326400 | -21.19725700 |
| C | -3.73611000 | 0.77463900  | -21.12015300 |
| H | -4.16121300 | -0.22764500 | -21.11235800 |
| H | -2.64083100 | 0.67247500  | -21.19725700 |
| C | -1.19719900 | 3.62288600  | -21.12015300 |
| H | -2.27775300 | 3.48989400  | -21.11235800 |
| H | -0.73803500 | 2.62326400  | -21.19725700 |
| C | -2.53891200 | -2.84824700 | -21.12015300 |
| H | -1.88346000 | -3.71753800 | -21.11235800 |
| H | -1.90279500 | -1.95078900 | -21.19725700 |
| C | 2.93494800  | 3.64961000  | -18.84972100 |
| O | 1.98504300  | 4.44310600  | -18.90992000 |
| C | 4.62812900  | -0.71693500 | -18.84972100 |
| O | 4.84036400  | 0.50245600  | -18.90992000 |
| C | 1.69318100  | -4.36654500 | -18.84972100 |
| O | 2.85532200  | -3.94065100 | -18.90992000 |
| C | -4.62812900 | 0.71693500  | -18.84972100 |
| O | -4.84036400 | -0.50245600 | -18.90992000 |
| C | -1.69318100 | 4.36654500  | -18.84972100 |
| O | -2.85532200 | 3.94065100  | -18.90992000 |
| C | -2.93494800 | -3.64961000 | -18.84972100 |
| O | -1.98504300 | -4.44310600 | -18.90992000 |
| C | 3.80924500  | 3.54267200  | -17.60750300 |
| H | 4.43355000  | 2.64466600  | -17.66089400 |
| H | 4.48719200  | 4.40832500  | -17.62181600 |
| C | 4.97266700  | -1.52756700 | -17.60750300 |



|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 4.50712300  | -2.51723400 | -17.66089400 |
| H | 6.06131800  | -1.68185900 | -17.62181600 |
| C | 1.16342200  | -5.07023900 | -17.60750300 |
| H | 0.07357300  | -5.16190000 | -17.66089400 |
| H | 1.57412600  | -6.09018500 | -17.62181600 |
| C | -4.97266700 | 1.52756700  | -17.60750300 |
| H | -4.50712300 | 2.51723400  | -17.66089400 |
| H | -6.06131800 | 1.68185900  | -17.62181600 |
| C | -1.16342200 | 5.07023900  | -17.60750300 |
| H | -0.07357300 | 5.16190000  | -17.66089400 |
| H | -1.57412600 | 6.09018500  | -17.62181600 |
| C | -3.80924500 | -3.54267200 | -17.60750300 |
| H | -4.43355000 | -2.64466600 | -17.66089400 |
| H | -4.48719200 | -4.40832500 | -17.62181600 |
| N | 3.28966100  | 2.84225200  | -19.88406500 |
| N | 4.10629300  | -1.42780400 | -19.88406500 |
| N | 0.81663200  | -4.27005600 | -19.88406500 |
| N | -4.10629300 | 1.42780400  | -19.88406500 |
| N | -0.81663200 | 4.27005600  | -19.88406500 |
| N | -3.28966100 | -2.84225200 | -19.88406500 |
| H | 3.80656100  | -2.39030200 | -19.72042000 |
| H | -0.16678200 | -4.49173000 | -19.72042000 |
| H | 3.97334300  | 2.10142800  | -19.72042000 |
| H | -3.80656100 | 2.39030200  | -19.72042000 |
| H | 0.16678200  | 4.49173000  | -19.72042000 |
| H | -3.97334300 | -2.10142800 | -19.72042000 |
| N | 3.02036300  | 3.71530500  | -23.32948300 |
| N | 4.72773000  | -0.75805900 | -23.32948300 |
| N | 1.70736700  | -4.47336400 | -23.32948300 |
| N | -4.72773000 | 0.75805900  | -23.32948300 |
| N | -1.70736700 | 4.47336400  | -23.32948300 |
| N | -3.02036300 | -3.71530500 | -23.32948300 |
| C | 5.09252400  | -1.27369200 | -24.64113300 |
| H | 6.16177600  | -1.11368700 | -24.82896000 |
| H | 4.88004900  | -2.34128700 | -24.65766400 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| C | 3.64931100  | 3.77341000  | -24.64113300 |
| H | 4.04536900  | 4.77941100  | -24.82896000 |
| H | 4.46763900  | 3.05560300  | -24.65766400 |
| C | -1.44321300 | 5.04710100  | -24.64113300 |
| H | -0.41241000 | 5.39689000  | -24.65766400 |
| H | -2.11640600 | 5.89309800  | -24.82896000 |
| C | -5.09252400 | 1.27369200  | -24.64113300 |
| H | -6.16177600 | 1.11368700  | -24.82896000 |
| H | -4.88004900 | 2.34128700  | -24.65766400 |
| C | -3.64931100 | -3.77341000 | -24.64113300 |
| H | -4.46763900 | -3.05560300 | -24.65766400 |
| H | -4.04536900 | -4.77941100 | -24.82896000 |
| C | 1.44321300  | -5.04710100 | -24.64113300 |
| H | 2.11640600  | -5.89309800 | -24.82896000 |
| H | 0.41241000  | -5.39689000 | -24.65766400 |
| C | -2.62747600 | -3.44317500 | -25.72639000 |
| O | -2.70431900 | -2.50497300 | -26.50838600 |
| C | 4.29561500  | -0.55387400 | -25.72639000 |
| O | 3.52152900  | -1.08952200 | -26.50838600 |
| C | 2.62747600  | 3.44317500  | -25.72639000 |
| O | 2.70431900  | 2.50497300  | -26.50838600 |
| C | -1.66813900 | 3.99704900  | -25.72639000 |
| O | -0.81721100 | 3.59449500  | -26.50838600 |
| C | -4.29561500 | 0.55387400  | -25.72639000 |
| O | -3.52152900 | 1.08952200  | -26.50838600 |
| C | 1.66813900  | -3.99704900 | -25.72639000 |
| O | 0.81721100  | -3.59449500 | -26.50838600 |
| O | -1.61883100 | -4.30158600 | -25.70336000 |
| H | -0.83560600 | -3.98576300 | -26.24038500 |
| O | 4.53469800  | 0.74884500  | -25.70336000 |
| H | 3.86957500  | 1.26922600  | -26.24038500 |
| O | 1.61883100  | 4.30158600  | -25.70336000 |
| H | 0.83560600  | 3.98576300  | -26.24038500 |
| O | -2.91586800 | 3.55274200  | -25.70336000 |
| H | -3.03396900 | 2.71653800  | -26.24038500 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| O | -4.53469800 | -0.74884500 | -25.70336000 |
| H | -3.86957500 | -1.26922600 | -26.24038500 |
| O | 2.91586800  | -3.55274200 | -25.70336000 |
| H | 3.03396900  | -2.71653800 | -26.24038500 |
| C | 2.98557500  | 3.56316700  | -16.31262300 |
| C | 3.85018300  | 3.55349900  | -15.04621800 |
| H | 2.31338600  | 2.69330500  | -16.29951500 |
| H | 2.34274800  | 4.45118600  | -16.31910700 |
| C | 3.01556800  | 3.55802400  | -13.75904800 |
| H | 4.50379900  | 2.66892500  | -15.05370400 |
| H | 4.51885900  | 4.42708800  | -15.05282300 |
| C | -4.57858100 | 0.80400000  | -16.31262300 |
| C | -5.00251200 | 1.55760700  | -15.04621800 |
| H | -3.48916400 | 0.65679900  | -16.29951500 |
| H | -5.02621400 | -0.19671300 | -16.31910700 |
| C | -4.58912300 | 0.83254700  | -13.75904800 |
| H | -4.56325700 | 2.56594100  | -15.05370400 |
| H | -6.09340000 | 1.69990300  | -15.05282300 |
| C | 4.57858100  | -0.80400000 | -16.31262300 |
| C | 5.00251200  | -1.55760700 | -15.04621800 |
| H | 3.48916400  | -0.65679900 | -16.29951500 |
| H | 5.02621400  | 0.19671300  | -16.31910700 |
| C | 4.58912300  | -0.83254700 | -13.75904800 |
| H | 4.56325700  | -2.56594100 | -15.05370400 |
| H | 6.09340000  | -1.69990300 | -15.05282300 |
| C | 1.59300600  | -4.36716800 | -16.31262300 |
| C | 1.15232900  | -5.11110600 | -15.04621800 |
| H | 1.17577800  | -3.35010400 | -16.29951500 |
| H | 2.68346600  | -4.25447300 | -16.31910700 |
| C | 1.57355500  | -4.39057100 | -13.75904800 |
| H | 0.05945800  | -5.23486700 | -15.05370400 |
| H | 1.57454100  | -6.12699100 | -15.05282300 |
| C | -1.59300600 | 4.36716800  | -16.31262300 |
| C | -1.15232900 | 5.11110600  | -15.04621800 |
| H | -1.17577800 | 3.35010400  | -16.29951500 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | -2.68346600 | 4.25447300  | -16.31910700 |
| C | -1.57355500 | 4.39057100  | -13.75904800 |
| H | -0.05945800 | 5.23486700  | -15.05370400 |
| H | -1.57454100 | 6.12699100  | -15.05282300 |
| C | -2.98557500 | -3.56316700 | -16.31262300 |
| C | -3.85018300 | -3.55349900 | -15.04621800 |
| H | -2.31338600 | -2.69330500 | -16.29951500 |
| H | -2.34274800 | -4.45118600 | -16.31910700 |
| C | -3.01556800 | -3.55802400 | -13.75904800 |
| H | -4.50379900 | -2.66892500 | -15.05370400 |
| H | -4.51885900 | -4.42708800 | -15.05282300 |
| C | 3.46923100  | 2.80378600  | -5.19690000  |
| O | 4.44310200  | 2.04575000  | -5.11684100  |
| C | 4.16276500  | -1.60254900 | -5.19690000  |
| O | 3.99322300  | -2.82496400 | -5.11684100  |
| C | 0.69353500  | -4.40633500 | -5.19690000  |
| O | -0.44987900 | -4.87071400 | -5.11684100  |
| C | -4.16276500 | 1.60254900  | -5.19690000  |
| O | -3.99322300 | 2.82496400  | -5.11684100  |
| C | -0.69353500 | 4.40633500  | -5.19690000  |
| O | 0.44987900  | 4.87071400  | -5.11684100  |
| C | -3.46923100 | -2.80378600 | -5.19690000  |
| O | -4.44310200 | -2.04575000 | -5.11684100  |
| H | 2.32702900  | 4.29712600  | -4.36424000  |
| H | 4.88493500  | 0.13329600  | -4.36424000  |
| H | 2.55790600  | -4.16383000 | -4.36424000  |
| H | -4.88493500 | -0.13329600 | -4.36424000  |
| H | -2.55790600 | 4.16383000  | -4.36424000  |
| H | -2.32702900 | -4.29712600 | -4.36424000  |
| C | 2.52935100  | 2.77384900  | -6.40191500  |
| H | 1.86789100  | 3.63844400  | -6.39387600  |
| H | 1.90846400  | 1.86863100  | -6.30785600  |
| C | 3.66689900  | -0.80355700 | -6.40191500  |
| H | 4.08493000  | 0.20158100  | -6.39387600  |
| H | 2.57251400  | -0.71846200 | -6.30785600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.13754900  | -3.57740700 | -6.40191500 |
| H | 2.21704000  | -3.43686300 | -6.39387600 |
| H | 0.66405000  | -2.58709400 | -6.30785600 |
| C | -3.66689900 | 0.80355700  | -6.40191500 |
| H | -4.08493000 | -0.20158100 | -6.39387600 |
| H | -2.57251400 | 0.71846200  | -6.30785600 |
| C | -1.13754900 | 3.57740700  | -6.40191500 |
| H | -2.21704000 | 3.43686300  | -6.39387600 |
| H | -0.66405000 | 2.58709400  | -6.30785600 |
| C | -2.52935100 | -2.77384900 | -6.40191500 |
| H | -1.86789100 | -3.63844400 | -6.39387600 |
| H | -1.90846400 | -1.86863100 | -6.30785600 |
| C | 2.93015900  | 3.60964600  | -8.66814900 |
| O | 2.00196400  | 4.42816000  | -8.59708900 |
| C | 4.59112500  | -0.73276900 | -8.66814900 |
| O | 4.83588100  | 0.48032900  | -8.59708900 |
| C | 1.66096600  | -4.34241600 | -8.66814900 |
| O | 2.83391800  | -3.94783200 | -8.59708900 |
| C | -4.59112500 | 0.73276900  | -8.66814900 |
| O | -4.83588100 | -0.48032900 | -8.59708900 |
| C | -1.66096600 | 4.34241600  | -8.66814900 |
| O | -2.83391800 | 3.94783200  | -8.59708900 |
| C | -2.93015900 | -3.60964600 | -8.66814900 |
| O | -2.00196400 | -4.42816000 | -8.59708900 |
| C | 3.80620500  | 3.50686200  | -9.90991900 |
| H | 4.42678100  | 2.60609800  | -9.86268000 |
| H | 4.48689100  | 4.37012900  | -9.88865100 |
| C | 4.94013400  | -1.54283900 | -9.90991900 |
| H | 4.47033800  | -2.53065600 | -9.86268000 |
| H | 6.02808800  | -1.70069700 | -9.88865100 |
| C | 1.13392900  | -5.04970100 | -9.90991900 |
| H | 0.04355700  | -5.13675400 | -9.86268000 |
| H | 1.54119700  | -6.07082600 | -9.88865100 |
| C | -4.94013400 | 1.54283900  | -9.90991900 |
| H | -4.47033800 | 2.53065600  | -9.86268000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -6.02808800 | 1.70069700  | -9.88865100 |
| C | -1.13392900 | 5.04970100  | -9.90991900 |
| H | -0.04355700 | 5.13675400  | -9.86268000 |
| H | -1.54119700 | 6.07082600  | -9.88865100 |
| C | -3.80620500 | -3.50686200 | -9.90991900 |
| H | -4.42678100 | -2.60609800 | -9.86268000 |
| H | -4.48689100 | -4.37012900 | -9.88865100 |
| N | 3.25753300  | 2.76957600  | -7.65345400 |
| N | 4.02729000  | -1.43631900 | -7.65345400 |
| N | 0.76975700  | -4.20589500 | -7.65345400 |
| N | -4.02729000 | 1.43631900  | -7.65345400 |
| N | -0.76975700 | 4.20589500  | -7.65345400 |
| N | -3.25753300 | -2.76957600 | -7.65345400 |
| H | 3.73261600  | -2.40039300 | -7.82258100 |
| H | -0.21249400 | -4.43273700 | -7.82258100 |
| H | 3.94511000  | 2.03234400  | -7.82258100 |
| H | -3.73261600 | 2.40039300  | -7.82258100 |
| H | 0.21249400  | 4.43273700  | -7.82258100 |
| H | -3.94511000 | -2.03234400 | -7.82258100 |
| N | 3.13981600  | 3.69707800  | -4.23218400 |
| N | 4.77167200  | -0.87062100 | -4.23218400 |
| N | 1.63185600  | -4.56770000 | -4.23218400 |
| N | -4.77167200 | 0.87062100  | -4.23218400 |
| N | -1.63185600 | 4.56770000  | -4.23218400 |
| N | -3.13981600 | -3.69707800 | -4.23218400 |
| C | 5.32884000  | -1.51946400 | -3.06305700 |
| H | 6.41909300  | -1.64027300 | -3.16284700 |
| H | 4.90186100  | -2.52017800 | -2.99262200 |
| C | 3.98031400  | 3.85517900  | -3.06305700 |
| H | 4.63006400  | 4.73896100  | -3.16284700 |
| H | 4.63346900  | 2.98504700  | -2.99262200 |
| C | -1.34852500 | 5.37464300  | -3.06305700 |
| H | -0.26839200 | 5.50522500  | -2.99262200 |
| H | -1.78902800 | 6.37923400  | -3.16284700 |
| C | -5.32884000 | 1.51946400  | -3.06305700 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | -6.41909300 | 1.64027300  | -3.16284700  |
| H | -4.90186100 | 2.52017800  | -2.99262200  |
| C | -3.98031400 | -3.85517900 | -3.06305700  |
| H | -4.63346900 | -2.98504700 | -2.99262200  |
| H | -4.63006400 | -4.73896100 | -3.16284700  |
| C | 1.34852500  | -5.37464300 | -3.06305700  |
| H | 1.78902800  | -6.37923400 | -3.16284700  |
| H | 0.26839200  | -5.50522500 | -2.99262200  |
| C | -3.25280800 | -4.01587500 | -1.74306700  |
| O | -3.81320900 | -3.71772400 | -0.69330800  |
| C | 5.10425400  | -0.80907700 | -1.74306700  |
| O | 5.12624800  | -1.44347400 | -0.69330800  |
| C | 3.25280800  | 4.01587500  | -1.74306700  |
| O | 3.81320900  | 3.71772400  | -0.69330800  |
| C | -1.85144600 | 4.82495200  | -1.74306700  |
| O | -1.31303900 | 5.16119800  | -0.69330800  |
| C | -5.10425400 | 0.80907700  | -1.74306700  |
| O | -5.12624800 | 1.44347400  | -0.69330800  |
| C | 1.85144600  | -4.82495200 | -1.74306700  |
| O | 1.31303900  | -5.16119800 | -0.69330800  |
| O | -2.04664500 | -4.55139600 | -1.82541700  |
| H | -1.70648600 | -4.73599100 | -0.89814100  |
| O | 4.96494700  | 0.50325200  | -1.82541700  |
| H | 4.95473100  | 0.89013500  | -0.89814100  |
| O | 2.04664500  | 4.55139600  | -1.82541700  |
| H | 1.70648600  | 4.73599100  | -0.89814100  |
| O | -2.91830300 | 4.04814500  | -1.82541700  |
| H | -3.24824600 | 3.84585500  | -0.89814100  |
| O | -4.96494700 | -0.50325200 | -1.82541700  |
| H | -4.95473100 | -0.89013500 | -0.89814100  |
| O | 2.91830300  | -4.04814500 | -1.82541700  |
| H | 3.24824600  | -3.84585500 | -0.89814100  |
| C | 2.98372800  | 3.54098300  | -11.20549500 |
| C | 3.84921400  | 3.54100900  | -12.47135000 |
| H | 2.30943800  | 2.67285600  | -11.22715300 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 2.34341800  | 4.43075200  | -11.19147600 |
| H | 4.50156200  | 2.65547500  | -12.47119200 |
| H | 4.51911100  | 4.41355900  | -12.45651400 |
| C | -4.55844500 | 0.81349200  | -11.20549500 |
| C | -4.99121100 | 1.56301300  | -12.47135000 |
| H | -3.46948000 | 0.66360400  | -11.22715300 |
| H | -5.00885300 | -0.18591600 | -11.19147600 |
| H | -4.55049000 | 2.57073000  | -12.47119200 |
| H | -6.08181000 | 1.70688500  | -12.45651400 |
| C | 4.55844500  | -0.81349200 | -11.20549500 |
| C | 4.99121100  | -1.56301300 | -12.47135000 |
| H | 3.46948000  | -0.66360400 | -11.22715300 |
| H | 5.00885300  | 0.18591600  | -11.19147600 |
| H | 4.55049000  | -2.57073000 | -12.47119200 |
| H | 6.08181000  | -1.70688500 | -12.45651400 |
| C | 1.57471800  | -4.35447600 | -11.20549500 |
| C | 1.14199700  | -5.10402200 | -12.47135000 |
| H | 1.16004300  | -3.33646000 | -11.22715300 |
| H | 2.66543500  | -4.24483600 | -11.19147600 |
| H | 0.04892800  | -5.22620500 | -12.47119200 |
| H | 1.56269900  | -6.12044500 | -12.45651400 |
| C | -1.57471800 | 4.35447600  | -11.20549500 |
| C | -1.14199700 | 5.10402200  | -12.47135000 |
| H | -1.16004300 | 3.33646000  | -11.22715300 |
| H | -2.66543500 | 4.24483600  | -11.19147600 |
| H | -0.04892800 | 5.22620500  | -12.47119200 |
| H | -1.56269900 | 6.12044500  | -12.45651400 |
| C | -2.98372800 | -3.54098300 | -11.20549500 |
| C | -3.84921400 | -3.54100900 | -12.47135000 |
| H | -2.30943800 | -2.67285600 | -11.22715300 |
| H | -2.34341800 | -4.43075200 | -11.19147600 |
| H | -4.50156200 | -2.65547500 | -12.47119200 |
| H | -4.51911100 | -4.41355900 | -12.45651400 |
| H | 5.03057900  | 0.17530100  | -13.75504000 |
| H | 3.49873300  | -0.68588700 | -13.76350300 |



|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 2.34336300  | 2.68704800  | -13.76350300 |
| H | 2.36347400  | 4.44425900  | -13.75504000 |
| H | -1.15537100 | 3.37293600  | -13.76350300 |
| H | -2.66710400 | 4.26895800  | -13.75504000 |
| H | -3.49873300 | 0.68588700  | -13.76350300 |
| H | -5.03057900 | -0.17530100 | -13.75504000 |
| H | -2.36347400 | -4.44425900 | -13.75504000 |
| H | -2.34336300 | -2.68704800 | -13.76350300 |
| H | 2.66710400  | -4.26895800 | -13.75504000 |
| H | 1.15537100  | -3.37293600 | -13.76350300 |

### [HCONHCH<sub>2</sub>-COOH]<sub>4</sub> Dimer

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 2.55201100  | 0.67102900  | 5.18149600 |
| O | 3.10134400  | -0.43201000 | 5.20475800 |
| C | -0.67102900 | 2.55201100  | 5.18149600 |
| O | 0.43201000  | 3.10134400  | 5.20475800 |
| C | -2.55201100 | -0.67102900 | 5.18149600 |
| O | -3.10134400 | 0.43201000  | 5.20475800 |
| C | 0.67102900  | -2.55201100 | 5.18149600 |
| O | -0.43201000 | -3.10134400 | 5.20475800 |
| H | -2.43693600 | 2.11733800  | 4.29331200 |
| H | 2.11733800  | 2.43693600  | 4.29331200 |
| H | -2.11733800 | -2.43693600 | 4.29331200 |
| H | 2.43693600  | -2.11733800 | 4.29331200 |
| N | -1.60339100 | 2.69676500  | 4.21647300 |
| N | 2.69676500  | 1.60339100  | 4.21647300 |
| N | -2.69676500 | -1.60339100 | 4.21647300 |
| N | 1.60339100  | -2.69676500 | 4.21647300 |
| C | 3.54710700  | 1.38236600  | 3.06927100 |
| H | 4.49436500  | 1.93609100  | 3.15880800 |
| H | 3.80280800  | 0.32191500  | 3.02934100 |
| C | -1.38236600 | 3.54710700  | 3.06927100 |
| H | -1.93609100 | 4.49436500  | 3.15880800 |
| H | -0.32191500 | 3.80280800  | 3.02934100 |
| C | -3.54710700 | -1.38236600 | 3.06927100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.49436500 | -1.93609100 | 3.15880800  |
| H | -3.80280800 | -0.32191500 | 3.02934100  |
| C | 1.38236600  | -3.54710700 | 3.06927100  |
| H | 0.32191500  | -3.80280800 | 3.02934100  |
| H | 1.93609100  | -4.49436500 | 3.15880800  |
| C | -1.78267600 | 2.94977300  | 1.73410700  |
| O | -1.36990900 | 3.44351400  | 0.68881200  |
| C | 2.94977300  | 1.78267600  | 1.73410700  |
| O | 3.44351400  | 1.36990900  | 0.68881200  |
| C | -2.94977300 | -1.78267600 | 1.73410700  |
| O | -3.44351400 | -1.36990900 | 0.68881200  |
| C | 1.78267600  | -2.94977300 | 1.73410700  |
| O | 1.36990900  | -3.44351400 | 0.68881200  |
| O | -2.62687500 | 1.93501500  | 1.80443800  |
| H | -2.91833700 | 1.67675200  | 0.87669500  |
| O | 1.93501500  | 2.62687500  | 1.80443800  |
| H | 1.67675200  | 2.91833700  | 0.87669500  |
| O | -1.93501500 | -2.62687500 | 1.80443800  |
| H | -1.67675200 | -2.91833700 | 0.87669500  |
| O | 2.62687500  | -1.93501500 | 1.80443800  |
| H | 2.91833700  | -1.67675200 | 0.87669500  |
| C | -0.67102900 | -2.55201100 | -5.18149600 |
| O | 0.43201000  | -3.10134400 | -5.20475800 |
| C | -2.55201100 | 0.67102900  | -5.18149600 |
| O | -3.10134400 | -0.43201000 | -5.20475800 |
| C | 0.67102900  | 2.55201100  | -5.18149600 |
| O | -0.43201000 | 3.10134400  | -5.20475800 |
| C | 2.55201100  | -0.67102900 | -5.18149600 |
| O | 3.10134400  | 0.43201000  | -5.20475800 |
| H | -2.11733800 | 2.43693600  | -4.29331200 |
| H | -2.43693600 | -2.11733800 | -4.29331200 |
| H | 2.43693600  | 2.11733800  | -4.29331200 |
| H | 2.11733800  | -2.43693600 | -4.29331200 |
| N | -2.69676500 | 1.60339100  | -4.21647300 |
| N | -1.60339100 | -2.69676500 | -4.21647300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 1.60339100  | 2.69676500  | -4.21647300 |
| N | 2.69676500  | -1.60339100 | -4.21647300 |
| C | -1.38236600 | -3.54710700 | -3.06927100 |
| H | -1.93609100 | -4.49436500 | -3.15880800 |
| H | -0.32191500 | -3.80280800 | -3.02934100 |
| C | -3.54710700 | 1.38236600  | -3.06927100 |
| H | -4.49436500 | 1.93609100  | -3.15880800 |
| H | -3.80280800 | 0.32191500  | -3.02934100 |
| C | 1.38236600  | 3.54710700  | -3.06927100 |
| H | 1.93609100  | 4.49436500  | -3.15880800 |
| H | 0.32191500  | 3.80280800  | -3.02934100 |
| C | 3.54710700  | -1.38236600 | -3.06927100 |
| H | 3.80280800  | -0.32191500 | -3.02934100 |
| H | 4.49436500  | -1.93609100 | -3.15880800 |
| C | -2.94977300 | 1.78267600  | -1.73410700 |
| O | -3.44351400 | 1.36990900  | -0.68881200 |
| C | -1.78267600 | -2.94977300 | -1.73410700 |
| O | -1.36990900 | -3.44351400 | -0.68881200 |
| C | 1.78267600  | 2.94977300  | -1.73410700 |
| O | 1.36990900  | 3.44351400  | -0.68881200 |
| C | 2.94977300  | -1.78267600 | -1.73410700 |
| O | 3.44351400  | -1.36990900 | -0.68881200 |
| O | -1.93501500 | 2.62687500  | -1.80443800 |
| H | -1.67675200 | 2.91833700  | -0.87669500 |
| O | -2.62687500 | -1.93501500 | -1.80443800 |
| H | -2.91833700 | -1.67675200 | -0.87669500 |
| O | 2.62687500  | 1.93501500  | -1.80443800 |
| H | 2.91833700  | 1.67675200  | -0.87669500 |
| O | 1.93501500  | -2.62687500 | -1.80443800 |
| H | 1.67675200  | -2.91833700 | -0.87669500 |
| H | 1.87280000  | 1.01116500  | 5.97892500  |
| H | -1.01116500 | 1.87280000  | 5.97892500  |
| H | 1.01116500  | -1.87280000 | 5.97892500  |
| H | -1.87280000 | -1.01116500 | 5.97892500  |
| H | -1.01116500 | -1.87280000 | -5.97892500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.87280000  | -1.01116500 | -5.97892500 |
| H | -1.87280000 | 1.01116500  | -5.97892500 |
| H | 1.01116500  | 1.87280000  | -5.97892500 |

**[HCONHCH<sub>2</sub>-COOH]<sub>8</sub> Dimer**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.12138500 | 5.54308600  | -5.12209300 |
| O | -1.34779000 | 5.64707800  | -5.19812000 |
| C | -3.97776700 | 3.81098900  | -5.12194500 |
| O | -4.91507400 | 3.01320900  | -5.19594700 |
| C | 3.81766600  | 4.01700600  | -5.11805100 |
| O | 3.03213800  | 4.96458700  | -5.19395500 |
| C | 5.50413400  | 0.13683500  | -5.11840200 |
| O | 5.61154300  | 1.36299700  | -5.19248000 |
| H | 5.37274900  | 3.03509900  | -4.28122600 |
| H | 1.66855900  | 5.95887700  | -4.28230000 |
| H | -3.01394400 | 5.37918200  | -4.28917300 |
| H | 5.92160700  | -1.65650300 | -4.28660000 |
| N | 4.80340200  | 3.87785000  | -4.20928000 |
| N | 0.66852400  | 6.14426900  | -4.21020600 |
| N | -3.84986600 | 4.79999700  | -4.21498400 |
| N | 6.11037200  | -0.65719800 | -4.21337400 |
| C | 0.13774300  | 7.01094200  | -3.18132000 |
| H | 0.35380300  | 8.06820700  | -3.40261200 |
| H | -0.94551900 | 6.89636600  | -3.14858300 |
| C | 5.05265500  | 4.86735400  | -3.18429800 |
| H | 5.95428400  | 5.45741700  | -3.41317700 |
| H | 4.20888800  | 5.55601700  | -3.14714300 |
| C | 6.98815800  | -0.13161200 | -3.19108100 |
| H | 8.04246300  | -0.35211100 | -3.42186400 |
| H | 6.87816900  | 0.95200700  | -3.15563100 |
| C | -4.84130100 | 5.04008100  | -3.18986300 |
| H | -5.43326400 | 5.94153900  | -3.41419900 |
| H | -5.52766000 | 4.19420100  | -3.15900900 |
| C | 5.25550200  | 4.28667100  | -1.79612900 |
| O | 4.88671100  | 4.89471700  | -0.79661100 |
| C | 0.68787000  | 6.73823600  | -1.79262300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.00526800 | 6.90594700  | -0.79450400 |
| C | 6.72416900  | -0.68337400 | -1.80134400 |
| O | 6.89155100  | 0.01021800  | -0.80346700 |
| C | -4.26386700 | 5.23608100  | -1.79920000 |
| O | -4.87309200 | 4.85984800  | -0.80313800 |
| O | 5.90456000  | 3.13433500  | -1.78164200 |
| H | 6.08115300  | 2.85354100  | -0.83372100 |
| O | 1.96064900  | 6.37930400  | -1.77566400 |
| H | 2.28083500  | 6.30101700  | -0.82700200 |
| O | 6.37278400  | -1.95831100 | -1.78387300 |
| H | 6.30045000  | -2.28013400 | -0.83530700 |
| O | -3.11326700 | 5.88792300  | -1.77843100 |
| H | -2.83446800 | 6.05871800  | -0.82885400 |
| C | 0.12138500  | -5.54308600 | -5.12209300 |
| O | 1.34779000  | -5.64707800 | -5.19812000 |
| C | 3.97776700  | -3.81098900 | -5.12194500 |
| O | 4.91507400  | -3.01320900 | -5.19594700 |
| C | -3.81766600 | -4.01700600 | -5.11805100 |
| O | -3.03213800 | -4.96458700 | -5.19395500 |
| C | -5.50413400 | -0.13683500 | -5.11840200 |
| O | -5.61154300 | -1.36299700 | -5.19248000 |
| H | -5.37274900 | -3.03509900 | -4.28122600 |
| H | -1.66855900 | -5.95887700 | -4.28230000 |
| H | 3.01394400  | -5.37918200 | -4.28917300 |
| H | -5.92160700 | 1.65650300  | -4.28660000 |
| N | -4.80340200 | -3.87785000 | -4.20928000 |
| N | -0.66852400 | -6.14426900 | -4.21020600 |
| N | 3.84986600  | -4.79999700 | -4.21498400 |
| N | -6.11037200 | 0.65719800  | -4.21337400 |
| C | -0.13774300 | -7.01094200 | -3.18132000 |
| H | -0.35380300 | -8.06820700 | -3.40261200 |
| H | 0.94551900  | -6.89636600 | -3.14858300 |
| C | -5.05265500 | -4.86735400 | -3.18429800 |
| H | -5.95428400 | -5.45741700 | -3.41317700 |
| H | -4.20888800 | -5.55601700 | -3.14714300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -6.98815800 | 0.13161200  | -3.19108100 |
| H | -8.04246300 | 0.35211100  | -3.42186400 |
| H | -6.87816900 | -0.95200700 | -3.15563100 |
| C | 4.84130100  | -5.04008100 | -3.18986300 |
| H | 5.43326400  | -5.94153900 | -3.41419900 |
| H | 5.52766000  | -4.19420100 | -3.15900900 |
| C | -5.25550200 | -4.28667100 | -1.79612900 |
| O | -4.88671100 | -4.89471700 | -0.79661100 |
| C | -0.68787000 | -6.73823600 | -1.79262300 |
| O | 0.00526800  | -6.90594700 | -0.79450400 |
| C | -6.72416900 | 0.68337400  | -1.80134400 |
| O | -6.89155100 | -0.01021800 | -0.80346700 |
| C | 4.26386700  | -5.23608100 | -1.79920000 |
| O | 4.87309200  | -4.85984800 | -0.80313800 |
| O | -5.90456000 | -3.13433500 | -1.78164200 |
| H | -6.08115300 | -2.85354100 | -0.83372100 |
| O | -1.96064900 | -6.37930400 | -1.77566400 |
| H | -2.28083500 | -6.30101700 | -0.82700200 |
| O | -6.37278400 | 1.95831100  | -1.78387300 |
| H | -6.30045000 | 2.28013400  | -0.83530700 |
| O | 3.11326700  | -5.88792300 | -1.77843100 |
| H | 2.83446800  | -6.05871800 | -0.82885400 |
| C | -1.91376800 | 5.16139200  | 5.12135400  |
| O | -0.80856000 | 5.70320200  | 5.19473900  |
| C | 2.31639800  | 4.99504000  | 5.11802000  |
| O | 3.48461200  | 4.60741800  | 5.19239100  |
| C | -5.03835000 | 2.31430100  | 5.12234800  |
| O | -4.64618700 | 3.48094400  | 5.19849900  |
| C | -5.20721700 | -1.90682700 | 5.11801400  |
| O | -5.76446300 | -0.80936900 | 5.19385000  |
| H | -6.13219800 | 0.83754700  | 4.28320400  |
| H | -3.73647900 | 4.90225900  | 4.28948800  |
| H | 0.83622300  | 6.09011000  | 4.28618600  |
| H | -4.92381700 | -3.72368100 | 4.28085900  |
| N | -5.90456000 | 1.82880000  | 4.21081800  |

|   |             |             |            |
|---|-------------|-------------|------------|
| N | -2.87239100 | 5.43844800  | 4.21506400 |
| N | 1.82846800  | 5.86719100  | 4.21335400 |
| N | -5.47114300 | -2.86647400 | 4.20894800 |
| C | -2.69818300 | 6.44380400  | 3.19020800 |
| H | -3.28926900 | 7.34572400  | 3.41502500 |
| H | -1.64895000 | 6.73672500  | 3.15923100 |
| C | -6.48892900 | 2.66062900  | 3.18224600 |
| H | -7.54509000 | 2.88202600  | 3.40349500 |
| H | -5.95341900 | 3.60925400  | 3.15030200 |
| C | -6.47752600 | -2.70148000 | 3.18350800 |
| H | -7.37761500 | -3.29419800 | 3.41158300 |
| H | -6.77413600 | -1.65345800 | 3.14673100 |
| C | 2.65947800  | 6.46431900  | 3.19136400 |
| H | 2.87612600  | 7.51933200  | 3.42253000 |
| H | 3.61010800  | 5.93271000  | 3.15566400 |
| C | -6.45674300 | 2.04806500  | 1.79329800 |
| O | -6.33536600 | 2.75124400  | 0.79548700 |
| C | -3.10831200 | 5.99287700  | 1.79944200 |
| O | -2.52261600 | 6.40480000  | 0.80336600 |
| C | -6.02503800 | -3.11801600 | 1.79527700 |
| O | -6.43922800 | -2.53986500 | 0.79577000 |
| C | 2.04812200  | 6.44180900  | 1.80165200 |
| O | 2.75116000  | 6.32163000  | 0.80361800 |
| O | -6.63268900 | 0.73735700  | 1.77570200 |
| H | -6.68796300 | 0.41302000  | 0.82676300 |
| O | -4.16235000 | 5.19428000  | 1.77860500 |
| H | -4.43063200 | 5.00735700  | 0.82904200 |
| O | -5.22201500 | -4.16883700 | 1.78072600 |
| H | -5.03433600 | -4.44231500 | 0.83277800 |
| O | 0.73830600  | 6.62422800  | 1.78441700 |
| H | 0.41423800  | 6.68618800  | 0.83589700 |
| C | 1.91376800  | -5.16139200 | 5.12135400 |
| O | 0.80856000  | -5.70320200 | 5.19473900 |
| C | -2.31639800 | -4.99504000 | 5.11802000 |
| O | -3.48461200 | -4.60741800 | 5.19239100 |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 5.03835000  | -2.31430100 | 5.12234800 |
| O | 4.64618700  | -3.48094400 | 5.19849900 |
| C | 5.20721700  | 1.90682700  | 5.11801400 |
| O | 5.76446300  | 0.80936900  | 5.19385000 |
| H | 6.13219800  | -0.83754700 | 4.28320400 |
| H | 3.73647900  | -4.90225900 | 4.28948800 |
| H | -0.83622300 | -6.09011000 | 4.28618600 |
| H | 4.92381700  | 3.72368100  | 4.28085900 |
| N | 5.90456000  | -1.82880000 | 4.21081800 |
| N | 2.87239100  | -5.43844800 | 4.21506400 |
| N | -1.82846800 | -5.86719100 | 4.21335400 |
| N | 5.47114300  | 2.86647400  | 4.20894800 |
| C | 2.69818300  | -6.44380400 | 3.19020800 |
| H | 3.28926900  | -7.34572400 | 3.41502500 |
| H | 1.64895000  | -6.73672500 | 3.15923100 |
| C | 6.48892900  | -2.66062900 | 3.18224600 |
| H | 7.54509000  | -2.88202600 | 3.40349500 |
| H | 5.95341900  | -3.60925400 | 3.15030200 |
| C | 6.47752600  | 2.70148000  | 3.18350800 |
| H | 7.37761500  | 3.29419800  | 3.41158300 |
| H | 6.77413600  | 1.65345800  | 3.14673100 |
| C | -2.65947800 | -6.46431900 | 3.19136400 |
| H | -2.87612600 | -7.51933200 | 3.42253000 |
| H | -3.61010800 | -5.93271000 | 3.15566400 |
| C | 6.45674300  | -2.04806500 | 1.79329800 |
| O | 6.33536600  | -2.75124400 | 0.79548700 |
| C | 3.10831200  | -5.99287700 | 1.79944200 |
| O | 2.52261600  | -6.40480000 | 0.80336600 |
| C | 6.02503800  | 3.11801600  | 1.79527700 |
| O | 6.43922800  | 2.53986500  | 0.79577000 |
| C | -2.04812200 | -6.44180900 | 1.80165200 |
| O | -2.75116000 | -6.32163000 | 0.80361800 |
| O | 6.63268900  | -0.73735700 | 1.77570200 |
| H | 6.68796300  | -0.41302000 | 0.82676300 |
| O | 4.16235000  | -5.19428000 | 1.77860500 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.43063200  | -5.00735700 | 0.82904200  |
| O | 5.22201500  | 4.16883700  | 1.78072600  |
| H | 5.03433600  | 4.44231500  | 0.83277800  |
| O | -0.73830600 | -6.62422800 | 1.78441700  |
| H | -0.41423800 | -6.68618800 | 0.83589700  |
| H | 4.41824400  | 2.21503200  | 5.82034600  |
| H | -4.41824400 | -2.21503200 | 5.82034600  |
| H | 4.70784700  | -1.53634100 | 5.82687300  |
| H | -4.70784700 | 1.53634100  | 5.82687300  |
| H | 2.23073700  | -4.37642300 | 5.82434200  |
| H | -2.23073700 | 4.37642300  | 5.82434200  |
| H | -1.53880500 | -4.65472400 | 5.81822700  |
| H | 1.53880500  | 4.65472400  | 5.81822700  |
| H | -3.78662700 | -3.17037300 | -5.82018700 |
| H | 3.78662700  | 3.17037300  | -5.82018700 |
| H | -0.46099700 | -4.93093700 | -5.82698000 |
| H | 0.46099700  | 4.93093700  | -5.82698000 |
| H | 3.13162300  | -3.78964500 | -5.82508100 |
| H | -3.13162300 | 3.78964500  | -5.82508100 |
| H | 4.88396500  | -0.44189300 | -5.81927800 |
| H | -4.88396500 | 0.44189300  | -5.81927800 |

### [HCONHCH<sub>2</sub>-COOH]<sub>10</sub> Dimer

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 6.43749100  | -2.62555700 | 5.05510200 |
| O | 7.00051500  | -1.53137000 | 5.12953700 |
| C | 6.78889700  | 1.67632000  | 5.05493100 |
| O | 6.60864800  | 2.89355000  | 5.13130600 |
| C | 3.64530000  | -5.91991600 | 5.05785700 |
| O | 4.73934700  | -5.35665100 | 5.13247100 |
| C | -4.53622600 | -5.35242700 | 5.05623300 |
| O | -3.67051900 | -6.22688500 | 5.13270700 |
| C | -0.54004400 | -6.97118200 | 5.05845100 |
| O | 0.67582600  | -7.16025100 | 5.13471600 |
| H | 2.36701400  | -7.27012300 | 4.26840600 |
| H | 6.18545400  | -4.46906800 | 4.26859000 |
| H | 7.65564000  | 0.03270000  | 4.26219400 |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | -6.20386700 | -4.53730900 | 4.25912300 |
| H | -2.36604900 | -7.30532800 | 4.26175100 |
| N | -1.38208100 | -7.56393700 | 4.18863800 |
| N | 3.31503900  | -6.90102500 | 4.19448200 |
| N | 6.74244600  | -3.61773400 | 4.19506100 |
| N | 7.61063200  | 1.04911300  | 4.18989600 |
| N | -5.56548200 | -5.32948500 | 4.18617800 |
| C | 7.80729800  | -3.50079000 | 3.22257400 |
| H | 8.66935600  | -4.12580200 | 3.50392500 |
| H | 8.14228000  | -2.46468400 | 3.18912000 |
| C | 4.24737800  | -7.42103700 | 3.21808900 |
| H | 4.58343800  | -8.43319700 | 3.49297000 |
| H | 5.12394900  | -6.77482400 | 3.18809700 |
| C | -0.93143300 | -8.52573400 | 3.20644000 |
| H | 0.15758900  | -8.51606800 | 3.17682500 |
| H | -1.25242800 | -9.54451700 | 3.47489000 |
| C | -5.77310600 | -6.37113100 | 3.20386400 |
| H | -6.63273200 | -7.00417000 | 3.47472800 |
| H | -4.88848900 | -7.00616700 | 3.17060900 |
| C | 8.40169600  | 1.76650700  | 3.21374000 |
| H | 9.46706200  | 1.76898100  | 3.49311500 |
| H | 8.06368900  | 2.80155500  | 3.17744600 |
| C | 3.67719200  | -7.51481500 | 1.81308100 |
| O | 4.36825300  | -7.27536700 | 0.82842100 |
| C | 7.40367900  | -3.91637000 | 1.81817200 |
| O | 7.82236100  | -3.31920500 | 0.83201500 |
| C | -1.44794800 | -8.25923300 | 1.80286900 |
| O | -0.74940400 | -8.47086300 | 0.81712400 |
| C | -6.03755100 | -5.84949100 | 1.80186100 |
| O | -5.59981000 | -6.42972100 | 0.81387000 |
| C | 8.31718600  | 1.18847000  | 1.81146900 |
| O | 8.30804000  | 1.91455100  | 0.82298200 |
| O | -2.70483600 | -7.84915000 | 1.76365600 |
| H | -3.00910700 | -7.76358900 | 0.81082300 |
| O | 2.42093200  | -7.92663200 | 1.77184300 |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | 2.12703800  | -8.03976800 | 0.81866600 |
| O | 6.63039300  | -4.98882500 | 1.77965800 |
| H | 6.46072700  | -5.25692500 | 0.82726800 |
| O | -6.81280200 | -4.77835700 | 1.76673100 |
| H | -7.01172000 | -4.52885100 | 0.81488800 |
| O | 8.31667800  | -0.13383500 | 1.77718600 |
| H | 8.33643700  | -0.45343900 | 0.82577700 |
| C | -6.43749100 | 2.62555700  | 5.05510200 |
| O | -7.00051500 | 1.53137000  | 5.12953700 |
| C | -6.78889700 | -1.67632000 | 5.05493100 |
| O | -6.60864800 | -2.89355000 | 5.13130600 |
| C | -3.64530000 | 5.91991600  | 5.05785700 |
| O | -4.73934700 | 5.35665100  | 5.13247100 |
| C | 4.53622600  | 5.35242700  | 5.05623300 |
| O | 3.67051900  | 6.22688500  | 5.13270700 |
| C | 0.54004400  | 6.97118200  | 5.05845100 |
| O | -0.67582600 | 7.16025100  | 5.13471600 |
| H | -2.36701400 | 7.27012300  | 4.26840600 |
| H | -6.18545400 | 4.46906800  | 4.26859000 |
| H | -7.65564000 | -0.03270000 | 4.26219400 |
| H | 6.20386700  | 4.53730900  | 4.25912300 |
| H | 2.36604900  | 7.30532800  | 4.26175100 |
| N | 1.38208100  | 7.56393700  | 4.18863800 |
| N | -3.31503900 | 6.90102500  | 4.19448200 |
| N | -6.74244600 | 3.61773400  | 4.19506100 |
| N | -7.61063200 | -1.04911300 | 4.18989600 |
| N | 5.56548200  | 5.32948500  | 4.18617800 |
| C | -7.80729800 | 3.50079000  | 3.22257400 |
| H | -8.66935600 | 4.12580200  | 3.50392500 |
| H | -8.14228000 | 2.46468400  | 3.18912000 |
| C | -4.24737800 | 7.42103700  | 3.21808900 |
| H | -4.58343800 | 8.43319700  | 3.49297000 |
| H | -5.12394900 | 6.77482400  | 3.18809700 |
| C | 0.93143300  | 8.52573400  | 3.20644000 |
| H | -0.15758900 | 8.51606800  | 3.17682500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.25242800  | 9.54451700  | 3.47489000  |
| C | 5.77310600  | 6.37113100  | 3.20386400  |
| H | 6.63273200  | 7.00417000  | 3.47472800  |
| H | 4.88848900  | 7.00616700  | 3.17060900  |
| C | -8.40169600 | -1.76650700 | 3.21374000  |
| H | -9.46706200 | -1.76898100 | 3.49311500  |
| H | -8.06368900 | -2.80155500 | 3.17744600  |
| C | -3.67719200 | 7.51481500  | 1.81308100  |
| O | -4.36825300 | 7.27536700  | 0.82842100  |
| C | -7.40367900 | 3.91637000  | 1.81817200  |
| O | -7.82236100 | 3.31920500  | 0.83201500  |
| C | 1.44794800  | 8.25923300  | 1.80286900  |
| O | 0.74940400  | 8.47086300  | 0.81712400  |
| C | 6.03755100  | 5.84949100  | 1.80186100  |
| O | 5.59981000  | 6.42972100  | 0.81387000  |
| C | -8.31718600 | -1.18847000 | 1.81146900  |
| O | -8.30804000 | -1.91455100 | 0.82298200  |
| O | 2.70483600  | 7.84915000  | 1.76365600  |
| H | 3.00910700  | 7.76358900  | 0.81082300  |
| O | -2.42093200 | 7.92663200  | 1.77184300  |
| H | -2.12703800 | 8.03976800  | 0.81866600  |
| O | -6.63039300 | 4.98882500  | 1.77965800  |
| H | -6.46072700 | 5.25692500  | 0.82726800  |
| O | 6.81280200  | 4.77835700  | 1.76673100  |
| H | 7.01172000  | 4.52885100  | 0.81488800  |
| O | -8.31667800 | 0.13383500  | 1.77718600  |
| H | -8.33643700 | 0.45343900  | 0.82577700  |
| C | 5.15687000  | -4.73444700 | -5.05718900 |
| O | 4.39875900  | -5.70366800 | -5.13334200 |
| C | 1.38208100  | -6.82383600 | -5.05854000 |
| O | 0.19818200  | -7.15920700 | -5.13425300 |
| C | 6.96528600  | -0.82103900 | -5.05528400 |
| O | 6.93194300  | -2.05107800 | -5.13205400 |
| C | 2.90540800  | 6.31224800  | -5.05659600 |
| O | 4.06268600  | 5.89400100  | -5.13086500 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 6.09503700 | 3.40274800  | -5.05483500 |
| O | 6.79267400 | 2.38907100  | -5.12998500 |
| H | 7.62558500 | 0.91405900  | -4.25886600 |
| H | 6.71783800 | -3.72986100 | -4.26049000 |
| H | 3.23666300 | -6.93636200 | -4.26585700 |
| H | 1.46536900 | 7.49030900  | -4.26992400 |
| H | 5.60954700 | 5.19758100  | -4.26483100 |
| N | 6.26971800 | 4.42349900  | -4.19197200 |
| N | 7.70199700 | -0.10047600 | -4.18642000 |
| N | 6.17653100 | -4.59128000 | -4.18728300 |
| N | 2.29174100 | -7.31347000 | -4.19263200 |
| N | 2.45291400 | 7.24591800  | -4.19599100 |
| C | 6.50462300 | -5.60095600 | -3.20453400 |
| H | 7.43461800 | -6.12631200 | -3.47312400 |
| H | 5.70244700 | -6.33752700 | -3.17395700 |
| C | 8.56767800 | -0.71858300 | -3.20571800 |
| H | 9.62722300 | -0.59385200 | -3.47931600 |
| H | 8.35545600 | -1.78659800 | -3.17100100 |
| C | 7.33864800 | 4.43988700  | -3.21705400 |
| H | 7.79866500 | 3.45299100  | -3.18113700 |
| H | 8.11808600 | 5.16574400  | -3.49746000 |
| C | 3.31209400 | 7.88467800  | -3.22282800 |
| H | 3.51674000 | 8.93002300  | -3.50267500 |
| H | 4.26347900 | 7.35488600  | -3.19058700 |
| C | 1.96372700 | -8.32774200 | -3.21456700 |
| H | 2.40828600 | -9.29778700 | -3.48725400 |
| H | 0.88189100 | -8.45285100 | -3.18511800 |
| C | 8.40760100 | -0.15559900 | -1.80392200 |
| O | 8.48403500 | -0.87765500 | -0.81539600 |
| C | 6.70081800 | -5.05254900 | -1.80148800 |
| O | 6.33588900 | -5.68354900 | -0.81502900 |
| C | 6.88359700 | 4.80449200  | -1.81430700 |
| O | 7.37233400 | 4.26652500  | -0.82631500 |
| C | 2.73428700 | 7.91155500  | -1.81805000 |
| O | 3.44857900 | 7.75998200  | -0.83252400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.44362500  | -8.00495000 | -1.80979600 |
| O | 1.77518000  | -8.30166500 | -0.82512200 |
| O | 5.98168200  | 5.77142000  | -1.77915600 |
| H | 5.77846900  | 6.01817500  | -0.82756800 |
| O | 8.24498800  | 1.15665800  | -1.76969000 |
| H | 8.22168800  | 1.47561400  | -0.81811200 |
| O | 7.33864800  | -3.89442700 | -1.76354300 |
| H | 7.50320000  | -3.62351500 | -0.81102800 |
| O | 1.43720900  | 8.16759000  | -1.77835900 |
| H | 1.13093200  | 8.24661600  | -0.82564700 |
| O | 3.64200200  | -7.44667600 | -1.76858300 |
| H | 3.93332700  | -7.32742900 | -0.81533100 |
| C | -5.15687000 | 4.73444700  | -5.05718900 |
| O | -4.39875900 | 5.70366800  | -5.13334200 |
| C | -1.38208100 | 6.82383600  | -5.05854000 |
| O | -0.19818200 | 7.15920700  | -5.13425300 |
| C | -6.96528600 | 0.82103900  | -5.05528400 |
| O | -6.93194300 | 2.05107800  | -5.13205400 |
| C | -2.90540800 | -6.31224800 | -5.05659600 |
| O | -4.06268600 | -5.89400100 | -5.13086500 |
| C | -6.09503700 | -3.40274800 | -5.05483500 |
| O | -6.79267400 | -2.38907100 | -5.12998500 |
| H | -7.62558500 | -0.91405900 | -4.25886600 |
| H | -6.71783800 | 3.72986100  | -4.26049000 |
| H | -3.23666300 | 6.93636200  | -4.26585700 |
| H | -1.46536900 | -7.49030900 | -4.26992400 |
| H | -5.60954700 | -5.19758100 | -4.26483100 |
| N | -6.26971800 | -4.42349900 | -4.19197200 |
| N | -7.70199700 | 0.10047600  | -4.18642000 |
| N | -6.17653100 | 4.59128000  | -4.18728300 |
| N | -2.29174100 | 7.31347000  | -4.19263200 |
| N | -2.45291400 | -7.24591800 | -4.19599100 |
| C | -6.50462300 | 5.60095600  | -3.20453400 |
| H | -7.43461800 | 6.12631200  | -3.47312400 |
| H | -5.70244700 | 6.33752700  | -3.17395700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -8.56767800 | 0.71858300  | -3.20571800 |
| H | -9.62722300 | 0.59385200  | -3.47931600 |
| H | -8.35545600 | 1.78659800  | -3.17100100 |
| C | -7.33864800 | -4.43988700 | -3.21705400 |
| H | -7.79866500 | -3.45299100 | -3.18113700 |
| H | -8.11808600 | -5.16574400 | -3.49746000 |
| C | -3.31209400 | -7.88467800 | -3.22282800 |
| H | -3.51674000 | -8.93002300 | -3.50267500 |
| H | -4.26347900 | -7.35488600 | -3.19058700 |
| C | -1.96372700 | 8.32774200  | -3.21456700 |
| H | -2.40828600 | 9.29778700  | -3.48725400 |
| H | -0.88189100 | 8.45285100  | -3.18511800 |
| C | -8.40760100 | 0.15559900  | -1.80392200 |
| O | -8.48403500 | 0.87765500  | -0.81539600 |
| C | -6.70081800 | 5.05254900  | -1.80148800 |
| O | -6.33588900 | 5.68354900  | -0.81502900 |
| C | -6.88359700 | -4.80449200 | -1.81430700 |
| O | -7.37233400 | -4.26652500 | -0.82631500 |
| C | -2.73428700 | -7.91155500 | -1.81805000 |
| O | -3.44857900 | -7.75998200 | -0.83252400 |
| C | -2.44362500 | 8.00495000  | -1.80979600 |
| O | -1.77518000 | 8.30166500  | -0.82512200 |
| O | -5.98168200 | -5.77142000 | -1.77915600 |
| H | -5.77846900 | -6.01817500 | -0.82756800 |
| O | -8.24498800 | -1.15665800 | -1.76969000 |
| H | -8.22168800 | -1.47561400 | -0.81811200 |
| O | -7.33864800 | 3.89442700  | -1.76354300 |
| H | -7.50320000 | 3.62351500  | -0.81102800 |
| O | -1.43720900 | -8.16759000 | -1.77835900 |
| H | -1.13093200 | -8.24661600 | -0.82564700 |
| O | -3.64200200 | 7.44667600  | -1.76858300 |
| H | -3.93332700 | 7.32742900  | -0.81533100 |
| H | 4.54877100  | 4.48015000  | 5.72690600  |
| H | 6.27783800  | 0.96537900  | 5.72140400  |
| H | 5.60514900  | -2.90244400 | 5.71946300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.80840500  | -5.66436600 | 5.72505800  |
| H | -1.06803100 | -6.27688800 | 5.72929500  |
| H | 1.06803100  | 6.27688800  | 5.72929500  |
| H | -2.80840500 | 5.66436600  | 5.72505800  |
| H | -5.60514900 | 2.90244400  | 5.71946300  |
| H | -6.27783800 | -0.96537900 | 5.72140400  |
| H | -4.54877100 | -4.48015000 | 5.72690600  |
| H | -2.10748500 | -5.94891900 | -5.72155200 |
| H | -5.23569100 | -3.57325200 | -5.72061500 |
| H | -6.37656000 | 0.17602000  | -5.72472800 |
| H | -5.06771000 | 3.86694200  | -5.72825700 |
| H | -1.82030200 | 6.06735900  | -5.72679500 |
| H | 2.10748500  | 5.94891900  | -5.72155200 |
| H | 5.23569100  | 3.57325200  | -5.72061500 |
| H | 6.37656000  | -0.17602000 | -5.72472800 |
| H | 5.06771000  | -3.86694200 | -5.72825700 |
| H | 1.82030200  | -6.06735900 | -5.72679500 |

### **[HCONHCH<sub>2</sub>-COOH]<sub>16</sub> Dimer**

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -6.32973500 | 9.47311800  | 4.88114100 |
| O | -7.38439400 | 8.83894300  | 4.94502600 |
| C | -2.22270700 | 11.17430400 | 4.88114100 |
| O | -3.43977300 | 10.99200300 | 4.94502600 |
| H | -0.57472500 | 12.12395700 | 4.19719300 |
| H | -5.17061400 | 10.98113800 | 4.19719300 |
| N | -1.59258300 | 12.09483300 | 4.12425800 |
| N | -6.09984700 | 10.56471300 | 4.12425800 |
| C | -7.10575000 | 11.13810700 | 3.25455000 |
| H | -7.43467700 | 12.11903200 | 3.63029700 |
| H | -7.96909200 | 10.47511900 | 3.22713500 |
| C | -2.30248700 | 13.00952200 | 3.25455000 |
| H | -2.23099400 | 14.04165400 | 3.63029700 |
| H | -3.35382600 | 12.72738800 | 3.22713500 |
| C | -1.77361300 | 13.01222000 | 1.82892300 |
| O | -2.52666300 | 13.01052300 | 0.86128400 |
| C | -6.61816600 | 11.34299100 | 1.82892300 |



|   |             |             |            |
|---|-------------|-------------|------------|
| O | -7.31324400 | 11.05324400 | 0.86128400 |
| O | -0.45361300 | 13.06478100 | 1.75905700 |
| H | -0.15733900 | 13.11126100 | 0.80202200 |
| O | -5.41875900 | 11.89669300 | 1.75905700 |
| H | -5.16282400 | 12.05301500 | 0.80202200 |
| C | 2.22270700  | 11.17430400 | 4.88114100 |
| O | 1.02852100  | 11.47163100 | 4.94502600 |
| C | 6.32973500  | 9.47311800  | 4.88114100 |
| O | 5.34023300  | 10.20480700 | 4.94502600 |
| H | 8.16654000  | 8.97932400  | 4.19719300 |
| H | 4.10866100  | 11.42101300 | 4.19719300 |
| N | 7.42621200  | 9.67846500  | 4.12425800 |
| N | 3.15713700  | 11.78362400 | 4.12425800 |
| C | 2.85130800  | 12.90035500 | 3.25455000 |
| H | 3.31233900  | 13.82656100 | 3.63029700 |
| H | 1.77202900  | 13.04202700 | 3.22713500 |
| C | 7.57101700  | 10.82722600 | 3.25455000 |
| H | 8.35139800  | 11.50649900 | 3.63029700 |
| H | 6.62810900  | 11.37113500 | 3.22713500 |
| C | 7.94689500  | 10.45516300 | 1.82892300 |
| O | 7.41320900  | 10.98645000 | 0.86128400 |
| C | 3.34095600  | 12.70045600 | 1.82892300 |
| O | 2.64457900  | 12.98706800 | 0.86128400 |
| O | 8.91744200  | 9.55894800  | 1.75905700 |
| H | 9.15980700  | 9.38231700  | 0.80202200 |
| O | 4.58059100  | 12.24387400 | 1.75905700 |
| H | 4.87210100  | 12.17343700 | 0.80202200 |
| C | 9.47311800  | 6.32973500  | 4.88114100 |
| O | 8.83894300  | 7.38439400  | 4.94502600 |
| C | 11.17430400 | 2.22270700  | 4.88114100 |
| O | 10.99200300 | 3.43977300  | 4.94502600 |
| H | 12.12395700 | 0.57472500  | 4.19719300 |
| H | 10.98113800 | 5.17061400  | 4.19719300 |
| N | 12.09483300 | 1.59258300  | 4.12425800 |
| N | 10.56471300 | 6.09984700  | 4.12425800 |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 11.13810700 | 7.10575000  | 3.25455000 |
| H | 12.11903200 | 7.43467700  | 3.63029700 |
| H | 10.47511900 | 7.96909200  | 3.22713500 |
| C | 13.00952200 | 2.30248700  | 3.25455000 |
| H | 14.04165400 | 2.23099400  | 3.63029700 |
| H | 12.72738800 | 3.35382600  | 3.22713500 |
| C | 13.01222000 | 1.77361300  | 1.82892300 |
| O | 13.01052300 | 2.52666300  | 0.86128400 |
| C | 11.34299100 | 6.61816600  | 1.82892300 |
| O | 11.05324400 | 7.31324400  | 0.86128400 |
| O | 13.06478100 | 0.45361300  | 1.75905700 |
| H | 13.11126100 | 0.15733900  | 0.80202200 |
| O | 11.89669300 | 5.41875900  | 1.75905700 |
| H | 12.05301500 | 5.16282400  | 0.80202200 |
| C | 11.17430400 | -2.22270700 | 4.88114100 |
| O | 11.47163100 | -1.02852100 | 4.94502600 |
| C | 9.47311800  | -6.32973500 | 4.88114100 |
| O | 10.20480700 | -5.34023300 | 4.94502600 |
| H | 8.97932400  | -8.16654000 | 4.19719300 |
| H | 11.42101300 | -4.10866100 | 4.19719300 |
| N | 9.67846500  | -7.42621200 | 4.12425800 |
| N | 11.78362400 | -3.15713700 | 4.12425800 |
| C | 12.90035500 | -2.85130800 | 3.25455000 |
| H | 13.82656100 | -3.31233900 | 3.63029700 |
| H | 13.04202700 | -1.77202900 | 3.22713500 |
| C | 10.82722600 | -7.57101700 | 3.25455000 |
| H | 11.50649900 | -8.35139800 | 3.63029700 |
| H | 11.37113500 | -6.62810900 | 3.22713500 |
| C | 10.45516300 | -7.94689500 | 1.82892300 |
| O | 10.98645000 | -7.41320900 | 0.86128400 |
| C | 12.70045600 | -3.34095600 | 1.82892300 |
| O | 12.98706800 | -2.64457900 | 0.86128400 |
| O | 9.55894800  | -8.91744200 | 1.75905700 |
| H | 9.38231700  | -9.15980700 | 0.80202200 |
| O | 12.24387400 | -4.58059100 | 1.75905700 |

|   |             |              |            |
|---|-------------|--------------|------------|
| H | 12.17343700 | -4.87210100  | 0.80202200 |
| C | 6.32973500  | -9.47311800  | 4.88114100 |
| O | 7.38439400  | -8.83894300  | 4.94502600 |
| C | 2.22270700  | -11.17430400 | 4.88114100 |
| O | 3.43977300  | -10.99200300 | 4.94502600 |
| H | 0.57472500  | -12.12395700 | 4.19719300 |
| H | 5.17061400  | -10.98113800 | 4.19719300 |
| N | 1.59258300  | -12.09483300 | 4.12425800 |
| N | 6.09984700  | -10.56471300 | 4.12425800 |
| C | 7.10575000  | -11.13810700 | 3.25455000 |
| H | 7.43467700  | -12.11903200 | 3.63029700 |
| H | 7.96909200  | -10.47511900 | 3.22713500 |
| C | 2.30248700  | -13.00952200 | 3.25455000 |
| H | 2.23099400  | -14.04165400 | 3.63029700 |
| H | 3.35382600  | -12.72738800 | 3.22713500 |
| C | 1.77361300  | -13.01222000 | 1.82892300 |
| O | 2.52666300  | -13.01052300 | 0.86128400 |
| C | 6.61816600  | -11.34299100 | 1.82892300 |
| O | 7.31324400  | -11.05324400 | 0.86128400 |
| O | 0.45361300  | -13.06478100 | 1.75905700 |
| H | 0.15733900  | -13.11126100 | 0.80202200 |
| O | 5.41875900  | -11.89669300 | 1.75905700 |
| H | 5.16282400  | -12.05301500 | 0.80202200 |
| C | -2.22270700 | -11.17430400 | 4.88114100 |
| O | -1.02852100 | -11.47163100 | 4.94502600 |
| C | -6.32973500 | -9.47311800  | 4.88114100 |
| O | -5.34023300 | -10.20480700 | 4.94502600 |
| H | -8.16654000 | -8.97932400  | 4.19719300 |
| H | -4.10866100 | -11.42101300 | 4.19719300 |
| N | -7.42621200 | -9.67846500  | 4.12425800 |
| N | -3.15713700 | -11.78362400 | 4.12425800 |
| C | -2.85130800 | -12.90035500 | 3.25455000 |
| H | -3.31233900 | -13.82656100 | 3.63029700 |
| H | -1.77202900 | -13.04202700 | 3.22713500 |
| C | -7.57101700 | -10.82722600 | 3.25455000 |

|   |              |              |            |
|---|--------------|--------------|------------|
| H | -8.35139800  | -11.50649900 | 3.63029700 |
| H | -6.62810900  | -11.37113500 | 3.22713500 |
| C | -7.94689500  | -10.45516300 | 1.82892300 |
| O | -7.41320900  | -10.98645000 | 0.86128400 |
| C | -3.34095600  | -12.70045600 | 1.82892300 |
| O | -2.64457900  | -12.98706800 | 0.86128400 |
| O | -8.91744200  | -9.55894800  | 1.75905700 |
| H | -9.15980700  | -9.38231700  | 0.80202200 |
| O | -4.58059100  | -12.24387400 | 1.75905700 |
| H | -4.87210100  | -12.17343700 | 0.80202200 |
| C | -9.47311800  | -6.32973500  | 4.88114100 |
| O | -8.83894300  | -7.38439400  | 4.94502600 |
| C | -11.17430400 | -2.22270700  | 4.88114100 |
| O | -10.99200300 | -3.43977300  | 4.94502600 |
| H | -12.12395700 | -0.57472500  | 4.19719300 |
| H | -10.98113800 | -5.17061400  | 4.19719300 |
| N | -12.09483300 | -1.59258300  | 4.12425800 |
| N | -10.56471300 | -6.09984700  | 4.12425800 |
| C | -11.13810700 | -7.10575000  | 3.25455000 |
| H | -12.11903200 | -7.43467700  | 3.63029700 |
| H | -10.47511900 | -7.96909200  | 3.22713500 |
| C | -13.00952200 | -2.30248700  | 3.25455000 |
| H | -14.04165400 | -2.23099400  | 3.63029700 |
| H | -12.72738800 | -3.35382600  | 3.22713500 |
| C | -13.01222000 | -1.77361300  | 1.82892300 |
| O | -13.01052300 | -2.52666300  | 0.86128400 |
| C | -11.34299100 | -6.61816600  | 1.82892300 |
| O | -11.05324400 | -7.31324400  | 0.86128400 |
| O | -13.06478100 | -0.45361300  | 1.75905700 |
| H | -13.11126100 | -0.15733900  | 0.80202200 |
| O | -11.89669300 | -5.41875900  | 1.75905700 |
| H | -12.05301500 | -5.16282400  | 0.80202200 |
| C | -11.17430400 | 2.22270700   | 4.88114100 |
| O | -11.47163100 | 1.02852100   | 4.94502600 |
| C | -9.47311800  | 6.32973500   | 4.88114100 |

|   |              |             |             |
|---|--------------|-------------|-------------|
| O | -10.20480700 | 5.34023300  | 4.94502600  |
| H | -8.97932400  | 8.16654000  | 4.19719300  |
| H | -11.42101300 | 4.10866100  | 4.19719300  |
| N | -9.67846500  | 7.42621200  | 4.12425800  |
| N | -11.78362400 | 3.15713700  | 4.12425800  |
| C | -12.90035500 | 2.85130800  | 3.25455000  |
| H | -13.82656100 | 3.31233900  | 3.63029700  |
| H | -13.04202700 | 1.77202900  | 3.22713500  |
| C | -10.82722600 | 7.57101700  | 3.25455000  |
| H | -11.50649900 | 8.35139800  | 3.63029700  |
| H | -11.37113500 | 6.62810900  | 3.22713500  |
| C | -10.45516300 | 7.94689500  | 1.82892300  |
| O | -10.98645000 | 7.41320900  | 0.86128400  |
| C | -12.70045600 | 3.34095600  | 1.82892300  |
| O | -12.98706800 | 2.64457900  | 0.86128400  |
| O | -9.55894800  | 8.91744200  | 1.75905700  |
| H | -9.38231700  | 9.15980700  | 0.80202200  |
| O | -12.24387400 | 4.58059100  | 1.75905700  |
| H | -12.17343700 | 4.87210100  | 0.80202200  |
| C | 10.61366400  | 4.14267600  | -4.88093800 |
| O | 11.11503400  | 3.01878500  | -4.94462000 |
| C | 8.22041400   | 7.88900700  | -4.88093800 |
| O | 9.11371300   | 7.04253300  | -4.94462000 |
| H | 7.41315900   | 9.61133900  | -4.19734200 |
| H | 10.52696600  | 6.04282600  | -4.19734200 |
| N | 8.23097600   | 9.00465400  | -4.12428000 |
| N | 11.05036200  | 5.16935800  | -4.12428000 |
| C | 12.20345600  | 5.06360400  | -3.25464800 |
| H | 13.03463100  | 5.67963900  | -3.63043800 |
| H | 12.53170200  | 4.02572500  | -3.22722400 |
| C | 9.33676600   | 9.34822100  | -3.25464800 |
| H | 9.86892500   | 10.23544000 | -3.63043800 |
| H | 10.03720500  | 8.51496000  | -3.22722400 |
| C | 8.90443100   | 9.65310800  | -1.82904900 |
| O | 9.51852300   | 9.21755300  | -0.86128100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 11.92070600 | 5.51073100  | -1.82904900 |
| O | 12.32137300 | 4.87332700  | -0.86128100 |
| O | 7.85469100  | 10.45513900 | -1.75936500 |
| H | 7.63802000  | 10.66256900 | -0.80234000 |
| O | 11.25779600 | 6.65342900  | -1.75936500 |
| H | 11.13699900 | 6.92798500  | -0.80234000 |
| C | 4.57568000  | 10.43430800 | -4.88093800 |
| O | 5.72491200  | 9.99411900  | -4.94462000 |
| C | 0.23434000  | 11.39108000 | -4.88093800 |
| O | 1.46454600  | 11.42419100 | -4.94462000 |
| H | -1.55434800 | 12.03813800 | -4.19734200 |
| H | 3.17076500  | 11.71661200 | -4.19734200 |
| N | -0.54707300 | 12.18743100 | -4.12428000 |
| N | 4.15849800  | 11.46907400 | -4.12428000 |
| C | 5.04863700  | 12.20965600 | -3.25464800 |
| H | 5.20076400  | 13.23298700 | -3.63043800 |
| H | 6.01463400  | 11.70786900 | -3.22722400 |
| C | -0.00810000 | 13.21228100 | -3.25464800 |
| H | -0.25916500 | 14.21593200 | -3.63043800 |
| H | 1.07639000  | 13.11836100 | -3.22722400 |
| C | -0.52939500 | 13.12216200 | -1.82904900 |
| O | 0.21281800  | 13.24840600 | -0.86128100 |
| C | 4.53253700  | 12.32588700 | -1.82904900 |
| O | 5.26656400  | 12.15848900 | -0.86128100 |
| O | -1.83879400 | 12.94700400 | -1.75936500 |
| H | -2.13867900 | 12.94047100 | -0.80234000 |
| O | 3.25578000  | 12.66514900 | -1.75936500 |
| H | 2.97622200  | 12.77387300 | -0.80234000 |
| C | -4.14267600 | 10.61366400 | -4.88093800 |
| O | -3.01878500 | 11.11503400 | -4.94462000 |
| C | -7.88900700 | 8.22041400  | -4.88093800 |
| O | -7.04253300 | 9.11371300  | -4.94462000 |
| H | -9.61133900 | 7.41315900  | -4.19734200 |
| H | -6.04282600 | 10.52696600 | -4.19734200 |
| N | -9.00465400 | 8.23097600  | -4.12428000 |

|   |              |             |             |
|---|--------------|-------------|-------------|
| N | -5.16935800  | 11.05036200 | -4.12428000 |
| C | -5.06360400  | 12.20345600 | -3.25464800 |
| H | -5.67963900  | 13.03463100 | -3.63043800 |
| H | -4.02572500  | 12.53170200 | -3.22722400 |
| C | -9.34822100  | 9.33676600  | -3.25464800 |
| H | -10.23544000 | 9.86892500  | -3.63043800 |
| H | -8.51496000  | 10.03720500 | -3.22722400 |
| C | -9.65310800  | 8.90443100  | -1.82904900 |
| O | -9.21755300  | 9.51852300  | -0.86128100 |
| C | -5.51073100  | 11.92070600 | -1.82904900 |
| O | -4.87332700  | 12.32137300 | -0.86128100 |
| O | -10.45513900 | 7.85469100  | -1.75936500 |
| H | -10.66256900 | 7.63802000  | -0.80234000 |
| O | -6.65342900  | 11.25779600 | -1.75936500 |
| H | -6.92798500  | 11.13699900 | -0.80234000 |
| C | -10.43430800 | 4.57568000  | -4.88093800 |
| O | -9.99411900  | 5.72491200  | -4.94462000 |
| C | -11.39108000 | 0.23434000  | -4.88093800 |
| O | -11.42419100 | 1.46454600  | -4.94462000 |
| H | -12.03813800 | -1.55434800 | -4.19734200 |
| H | -11.71661200 | 3.17076500  | -4.19734200 |
| N | -12.18743100 | -0.54707300 | -4.12428000 |
| N | -11.46907400 | 4.15849800  | -4.12428000 |
| C | -12.20965600 | 5.04863700  | -3.25464800 |
| H | -13.23298700 | 5.20076400  | -3.63043800 |
| H | -11.70786900 | 6.01463400  | -3.22722400 |
| C | -13.21228100 | -0.00810000 | -3.25464800 |
| H | -14.21593200 | -0.25916500 | -3.63043800 |
| H | -13.11836100 | 1.07639000  | -3.22722400 |
| C | -13.12216200 | -0.52939500 | -1.82904900 |
| O | -13.24840600 | 0.21281800  | -0.86128100 |
| C | -12.32588700 | 4.53253700  | -1.82904900 |
| O | -12.15848900 | 5.26656400  | -0.86128100 |
| O | -12.94700400 | -1.83879400 | -1.75936500 |
| H | -12.94047100 | -2.13867900 | -0.80234000 |

|   |              |              |             |
|---|--------------|--------------|-------------|
| O | -12.66514900 | 3.25578000   | -1.75936500 |
| H | -12.77387300 | 2.97622200   | -0.80234000 |
| C | -10.61366400 | -4.14267600  | -4.88093800 |
| O | -11.11503400 | -3.01878500  | -4.94462000 |
| C | -8.22041400  | -7.88900700  | -4.88093800 |
| O | -9.11371300  | -7.04253300  | -4.94462000 |
| H | -7.41315900  | -9.61133900  | -4.19734200 |
| H | -10.52696600 | -6.04282600  | -4.19734200 |
| N | -8.23097600  | -9.00465400  | -4.12428000 |
| N | -11.05036200 | -5.16935800  | -4.12428000 |
| C | -12.20345600 | -5.06360400  | -3.25464800 |
| H | -13.03463100 | -5.67963900  | -3.63043800 |
| H | -12.53170200 | -4.02572500  | -3.22722400 |
| C | -9.33676600  | -9.34822100  | -3.25464800 |
| H | -9.86892500  | -10.23544000 | -3.63043800 |
| H | -10.03720500 | -8.51496000  | -3.22722400 |
| C | -8.90443100  | -9.65310800  | -1.82904900 |
| O | -9.51852300  | -9.21755300  | -0.86128100 |
| C | -11.92070600 | -5.51073100  | -1.82904900 |
| O | -12.32137300 | -4.87332700  | -0.86128100 |
| O | -7.85469100  | -10.45513900 | -1.75936500 |
| H | -7.63802000  | -10.66256900 | -0.80234000 |
| O | -11.25779600 | -6.65342900  | -1.75936500 |
| H | -11.13699900 | -6.92798500  | -0.80234000 |
| C | -4.57568000  | -10.43430800 | -4.88093800 |
| O | -5.72491200  | -9.99411900  | -4.94462000 |
| C | -0.23434000  | -11.39108000 | -4.88093800 |
| O | -1.46454600  | -11.42419100 | -4.94462000 |
| H | 1.55434800   | -12.03813800 | -4.19734200 |
| H | -3.17076500  | -11.71661200 | -4.19734200 |
| N | 0.54707300   | -12.18743100 | -4.12428000 |
| N | -4.15849800  | -11.46907400 | -4.12428000 |
| C | -5.04863700  | -12.20965600 | -3.25464800 |
| H | -5.20076400  | -13.23298700 | -3.63043800 |
| H | -6.01463400  | -11.70786900 | -3.22722400 |



|   |             |              |             |
|---|-------------|--------------|-------------|
| C | 0.00810000  | -13.21228100 | -3.25464800 |
| H | 0.25916500  | -14.21593200 | -3.63043800 |
| H | -1.07639000 | -13.11836100 | -3.22722400 |
| C | 0.52939500  | -13.12216200 | -1.82904900 |
| O | -0.21281800 | -13.24840600 | -0.86128100 |
| C | -4.53253700 | -12.32588700 | -1.82904900 |
| O | -5.26656400 | -12.15848900 | -0.86128100 |
| O | 1.83879400  | -12.94700400 | -1.75936500 |
| H | 2.13867900  | -12.94047100 | -0.80234000 |
| O | -3.25578000 | -12.66514900 | -1.75936500 |
| H | -2.97622200 | -12.77387300 | -0.80234000 |
| C | 4.14267600  | -10.61366400 | -4.88093800 |
| O | 3.01878500  | -11.11503400 | -4.94462000 |
| C | 7.88900700  | -8.22041400  | -4.88093800 |
| O | 7.04253300  | -9.11371300  | -4.94462000 |
| H | 9.61133900  | -7.41315900  | -4.19734200 |
| H | 6.04282600  | -10.52696600 | -4.19734200 |
| N | 9.00465400  | -8.23097600  | -4.12428000 |
| N | 5.16935800  | -11.05036200 | -4.12428000 |
| C | 5.06360400  | -12.20345600 | -3.25464800 |
| H | 5.67963900  | -13.03463100 | -3.63043800 |
| H | 4.02572500  | -12.53170200 | -3.22722400 |
| C | 9.34822100  | -9.33676600  | -3.25464800 |
| H | 10.23544000 | -9.86892500  | -3.63043800 |
| H | 8.51496000  | -10.03720500 | -3.22722400 |
| C | 9.65310800  | -8.90443100  | -1.82904900 |
| O | 9.21755300  | -9.51852300  | -0.86128100 |
| C | 5.51073100  | -11.92070600 | -1.82904900 |
| O | 4.87332700  | -12.32137300 | -0.86128100 |
| O | 10.45513900 | -7.85469100  | -1.75936500 |
| H | 10.66256900 | -7.63802000  | -0.80234000 |
| O | 6.65342900  | -11.25779600 | -1.75936500 |
| H | 6.92798500  | -11.13699900 | -0.80234000 |
| C | 10.43430800 | -4.57568000  | -4.88093800 |
| O | 9.99411900  | -5.72491200  | -4.94462000 |

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | 11.39108000  | -0.23434000  | -4.88093800 |
| O | 11.42419100  | -1.46454600  | -4.94462000 |
| H | 12.03813800  | 1.55434800   | -4.19734200 |
| H | 11.71661200  | -3.17076500  | -4.19734200 |
| N | 12.18743100  | 0.54707300   | -4.12428000 |
| N | 11.46907400  | -4.15849800  | -4.12428000 |
| C | 12.20965600  | -5.04863700  | -3.25464800 |
| H | 13.23298700  | -5.20076400  | -3.63043800 |
| H | 11.70786900  | -6.01463400  | -3.22722400 |
| C | 13.21228100  | 0.00810000   | -3.25464800 |
| H | 14.21593200  | 0.25916500   | -3.63043800 |
| H | 13.11836100  | -1.07639000  | -3.22722400 |
| C | 13.12216200  | 0.52939500   | -1.82904900 |
| O | 13.24840600  | -0.21281800  | -0.86128100 |
| C | 12.32588700  | -4.53253700  | -1.82904900 |
| O | 12.15848900  | -5.26656400  | -0.86128100 |
| O | 12.94700400  | 1.83879400   | -1.75936500 |
| H | 12.94047100  | 2.13867900   | -0.80234000 |
| O | 12.66514900  | -3.25578000  | -1.75936500 |
| H | 12.77387300  | -2.97622200  | -0.80234000 |
| H | 10.34991300  | -2.65040500  | 5.47202200  |
| H | 4.41964500   | -9.72720800  | -5.47185000 |
| H | 10.57633900  | 1.51208600   | 5.47202200  |
| H | 0.36077800   | -10.67809400 | -5.47185000 |
| H | 9.19261300   | 5.44437500   | 5.47202200  |
| H | -3.75301400  | -10.00333600 | -5.47185000 |
| H | 6.40939500   | 8.54780700   | 5.47202200  |
| H | -7.29544400  | -7.80566100  | -5.47185000 |
| H | 2.65040500   | 10.34991300  | 5.47202200  |
| H | -9.72720800  | -4.41964500  | -5.47185000 |
| H | -1.51208600  | 10.57633900  | 5.47202200  |
| H | -10.67809400 | -0.36077800  | -5.47185000 |
| H | -5.44437500  | 9.19261300   | 5.47202200  |
| H | -10.00333600 | 3.75301400   | -5.47185000 |
| H | -8.54780700  | 6.40939500   | 5.47202200  |

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|---|--------------|--------------|-------------|
| H | -7.80566100  | 7.29544400   | -5.47185000 |
| H | -10.34991300 | 2.65040500   | 5.47202200  |
| H | -4.41964500  | 9.72720800   | -5.47185000 |
| H | -10.57633900 | -1.51208600  | 5.47202200  |
| H | -0.36077800  | 10.67809400  | -5.47185000 |
| H | -9.19261300  | -5.44437500  | 5.47202200  |
| H | 3.75301400   | 10.00333600  | -5.47185000 |
| H | -6.40939500  | -8.54780700  | 5.47202200  |
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| H | -2.65040500  | -10.34991300 | 5.47202200  |
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| H | 7.80566100   | -7.29544400  | -5.47185000 |