Optimized structure from the Gaussian03 logfile:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 4.466330 | 12.859865 | 3.576831 |
| 2 | 7 | 0 | 4.377325 | 7.221289 | 3.313898 |
| 3 | 6 | 0 | 4.458786 | 11.475706 | 3.534029 |
| 4 | 6 | 0 | 5.312485 | 10.701155 | 4.360882 |
| 5 | 1 | 0 | 5.993155 | 11.186190 | 5.050484 |
| 6 | 6 | 0 | 5.309884 | 9.315390 | 4.310621 |
| 7 | 1 | 0 | 5.968420 | 8.773863 | 4.984046 |
| 8 | 6 | 0 | 4.458089 | 8.612878 | 3.437370 |
| 9 | 6 | 0 | 3.586389 | 9.375996 | 2.642925 |
| 10 | 1 | 0 | 2.903091 | 8.847012 | 1.984956 |
| 11 | 6 | 0 | 3.587423 | 10.761998 | 2.674137 |
| 12 | 1 | 0 | 2.884348 | 11.291225 | 2.042379 |
| 13 | 6 | 0 | 5.267961 | 13.597073 | 4.549622 |
| 14 | 1 | 0 | 5.260961 | 13.062876 | 5.505700 |
| 15 | 1 | 0 | 4.760307 | 14.550095 | 4.738272 |
| 16 | 6 | 0 | 6.709145 | 13.864921 | 4.095324 |
| 17 | 1 | 0 | 7.247993 | 12.929194 | 3.916090 |
| 18 | 1 | 0 | 7.252763 | 14.435608 | 4.857620 |
| 19 | 1 | 0 | 6.723277 | 14.442901 | 3.164469 |
| 20 | 6 | 0 | 3.687226 | 13.660469 | 2.635995 |
| 21 | 1 | 0 | 3.684657 | 13.167951 | 1.657818 |
| 22 | 1 | 0 | 4.219585 | 14.607765 | 2.490538 |
| 23 | 6 | 0 | 2.251468 | 13.944753 | 3.096972 |
| 24 | 1 | 0 | 1.688510 | 13.016361 | 3.235695 |
| 25 | 1 | 0 | 1.725457 | 14.559415 | 2.356802 |
| 26 | 1 | 0 | 2.246844 | 14.484657 | 4.050615 |
| 27 | 7 | 0 | 5.046326 | 2.169753 | 3.411659 |
| 28 | 6 | 0 | 4.034929 | 2.964637 | 3.024199 |
| 29 | 1 | 0 | 3.152894 | 2.454761 | 2.639583 |
| 30 | 6 | 0 | 4.062899 | 4.352927 | 3.090849 |
| 31 | 1 | 0 | 3.219895 | 4.953430 | 2.766736 |
| 32 | 6 | 0 | 5.213886 | 4.984269 | 3.589539 |
| 33 | 6 | 0 | 6.273732 | 4.161516 | 3.995722 |
| 34 | 1 | 0 | 7.190201 | 4.593674 | 4.390550 |
| 35 | 6 | 0 | 6.139478 | 2.777751 | 3.887213 |
| 36 | 1 | 0 | 6.953032 | 2.123902 | 4.198523 |
| 37 | 6 | 0 | 5.326885 | 6.444356 | 3.688879 |
| 38 | 1 | 0 | 6.280260 | 6.817019 | 4.090960 |

Total energy:

SCF Done: E(RB+HF-LYP) = -785.385897044 A.U.