

Microplasma-Enabled Nanocarbon Assembly for Diameter-Selective Synthesis of Colloidal Graphene Quantum Dots

(Supporting information)

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S1. Materials and Chemicals

Platinum foil (0.1mm, 99.95 % pure) was purchased from Guv Team Co., Ltd (Taiwan). Stainless steel hollow capillarity tube was purchased from Swagelok (i.d.: 180 μm , length: 7cm). The carrier gas for the plasma was argon (Ar) with 99.99% purity. Sodium organosulfates ($\text{NaC}_n\text{H}_{2n+1}\text{SO}_4$) with $n=8, 10, 12, 14,$ and 18 were purchased from Acros organics (99% pure) and used without further purification. Deionized water was used in all experiments.

S2. Synthesis

The colloidal GQDs were synthesized in aqueous solutions using a direct current (dc) microplasma electrochemical reactor operated at ambient conditions. The experimental setup is shown in **Figure 1a**¹. The reactor consisted of a platinum (Pt) foil anode immersed in an electrolyte and a microplasma cathode. The distances between the anode and cathode and cathode to the liquid surface are approximately 3 cm and 1.5 mm, respectively. A flow of 25 sccm Ar was introduced in a hollow stainless steel capillary (i.d. = 180 μm) to facilitate the formation of a

microplasma. A dc power supply was used to ignite and maintain a stable plasma with constant currents of 5–9.6 mA. The process time was varying from 1 to 5 hr. The precursor was 1.25 mM sodium organosulfates ($\text{NaC}_n\text{H}_{2n+1}\text{SO}_4$) with $n=8, 10, 12, 14,$ and 18 aqueous solution. To increase the electrolyte conductivity, 0.25 mL of 0.1 M HCl aqueous solution was added into the 50 mL sodium organosulfates solution. The as-prepared GQD solution was purified using dialysis membrane (MWCO: 1 kD) for 24 hours.

S3. Materials characterizations

Ex situ characterizations of the as-produced samples were performed by absorbance spectroscopy, photoluminescence (PL), transmission electron microscopy (TEM), atomic force microscopy (AFM), microRaman, X-ray photoelectron spectroscopy (XPS) and Fourier-transform infrared spectroscopy (FTIR). Absorbance spectra of synthesized materials were recorded using JASCO, V676 absorbance spectrophotometer in a matched pair of quartz cuvette of path length 1 cm. The baseline correction was done using corresponding solvents during every spectral measurement. PL spectroscopy measurements were performed at room temperature on the liquid as-produced GQD dispersions. Excitation and emission spectra were obtained by a commercial spectrometer (Horiba Jobin Yvon Nanolog-3 spectrofluorometer) equipped with an InGaAs NIR detector and a 20 nm bandpass for both emission and excitation. The PL spectra were scaled according to the measured excitation power. TEM was performed using a Cold-field emission Cs-corrected TEM (JEOL ARM-200F, Japan) with 200 kV accelerating voltage. TEM samples were prepared from solution dry-casting of the colloidal solution on lacey carbon-coated copper grids (400 mesh, Ted Pella Inc.). AFM was carried out by Ardic instruments P-100 at a scanning frequency: 0.8 -1.0 Hz, scanning mode - constant contact Scanning and scanning area - $5 \times 5\mu\text{m}$ or $1 \times 1\mu\text{m}$. The samples were prepared by ethanol solution and spin coating on mica substrates. Micro Raman measurement was carried out at room temperature with a JASCO 5100 spectrometer (laser

excitation wavelength $\lambda=532$ nm). Thin film for as-purified GQDs was drop-coated on Si wafer and dried in ambient conditions for 24 hrs. The laser power was maintained at 0.1 mW to avoid heat generation by the laser. Silicon wafer was used to calibrate Raman shifts using the 520 cm^{-1} peak. FTIR was carried by a Nicolet FTIR-iS10 with ATR mode. The samples were dispersed by ethanol and film casted on the potassium bromide (KBr) pallets. XPS was additionally performed with thin film for as-purified GQDs drop-coated on Si wafer using a VG ESCA Scientific Theta Probe with a pass energy 50 eV, 53° take off angle, and a $400\text{ }\mu\text{m}$ beam size.

S5. TEM characterizations

Figure S1 shows a representative HRTEM image of as-produced GQD-N12, indicating spherical particle-like nanostructures with diameter around 5 nm. Moreover, 0.21 nm graphite lattice spacing was observed, confirming that the graphene lattice was existent in the GQD-N12. **Figure S3 (a)** shows additional representative TEM image of as-produced GQD-N18, showing particle-like nanostructures. The HRTEM images shown in **Figure S3 (b)** and **(c)** of GQD-N18 indicate particle diameters about 6.8 and 6.5 nm, respectively.

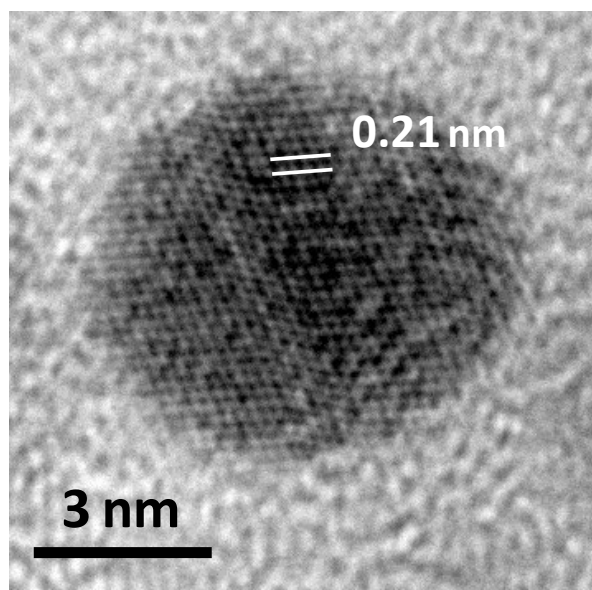


Figure S1. HRTEM image of as-produced colloidal GQD-N12 synthesized for 1 hr at a constant discharge current of 9.6 mA.

S6. MicroRaman spectroscopy analysis

Figure S2 shows the representative Raman spectra of as-purified GQD-N12 and commercial CVD-grown graphenes. The G and D bands can be observed at 1591.6 and 1344.7 cm^{-1} , respectively, with an I_D/I_G ratio of 1.15. The structural defects result from oxygenated function groups capped onto GQDs or vacancy sites in the basal planes or along the edges of GQDs. A small 2D band near 2780 nm is also observed and the intensity was compatible with CVD-grown few-layered graphenes, indicating the nano-sized few-layered graphene structures were existed in the as-produced GQD-N12.

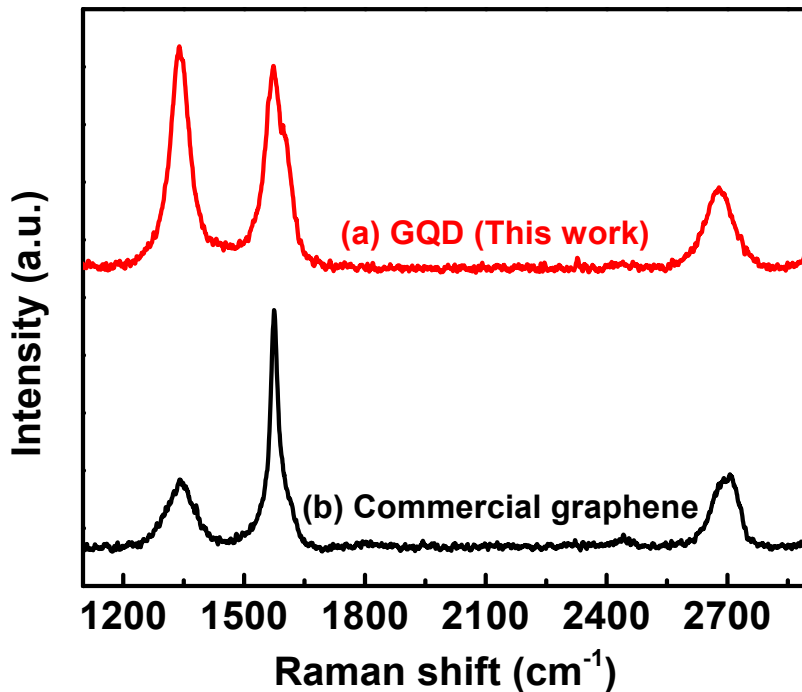


Figure S2. Micro Raman spectra of as-produced colloidal GQD-N12 synthesized for 1 hr at a constant discharge current of 9.6 mA and commercial CVD-grown graphenes.

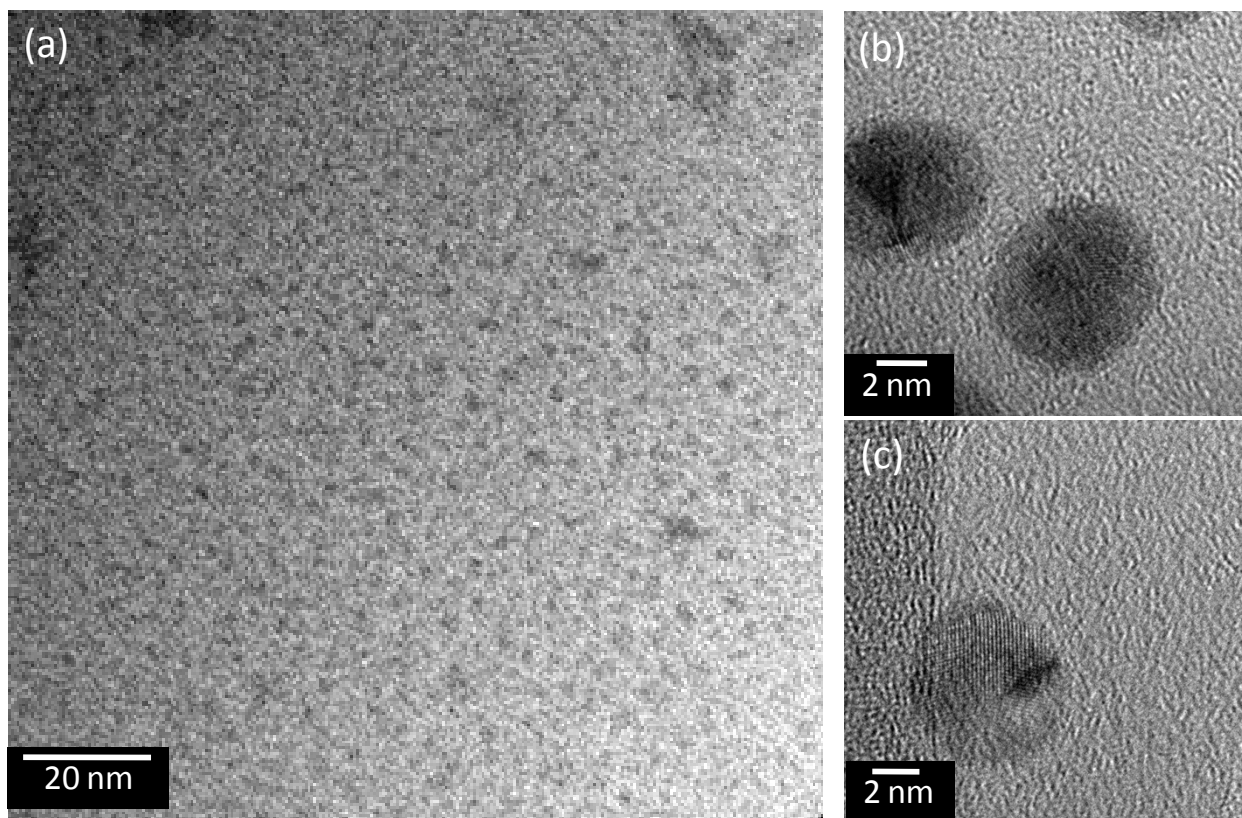


Figure S3. (a) TEM and (b) and (c) HRTEM image of as-produced colloidal GQD-N18 synthesized for 1 hr at a constant discharge current of 9.6 mA.

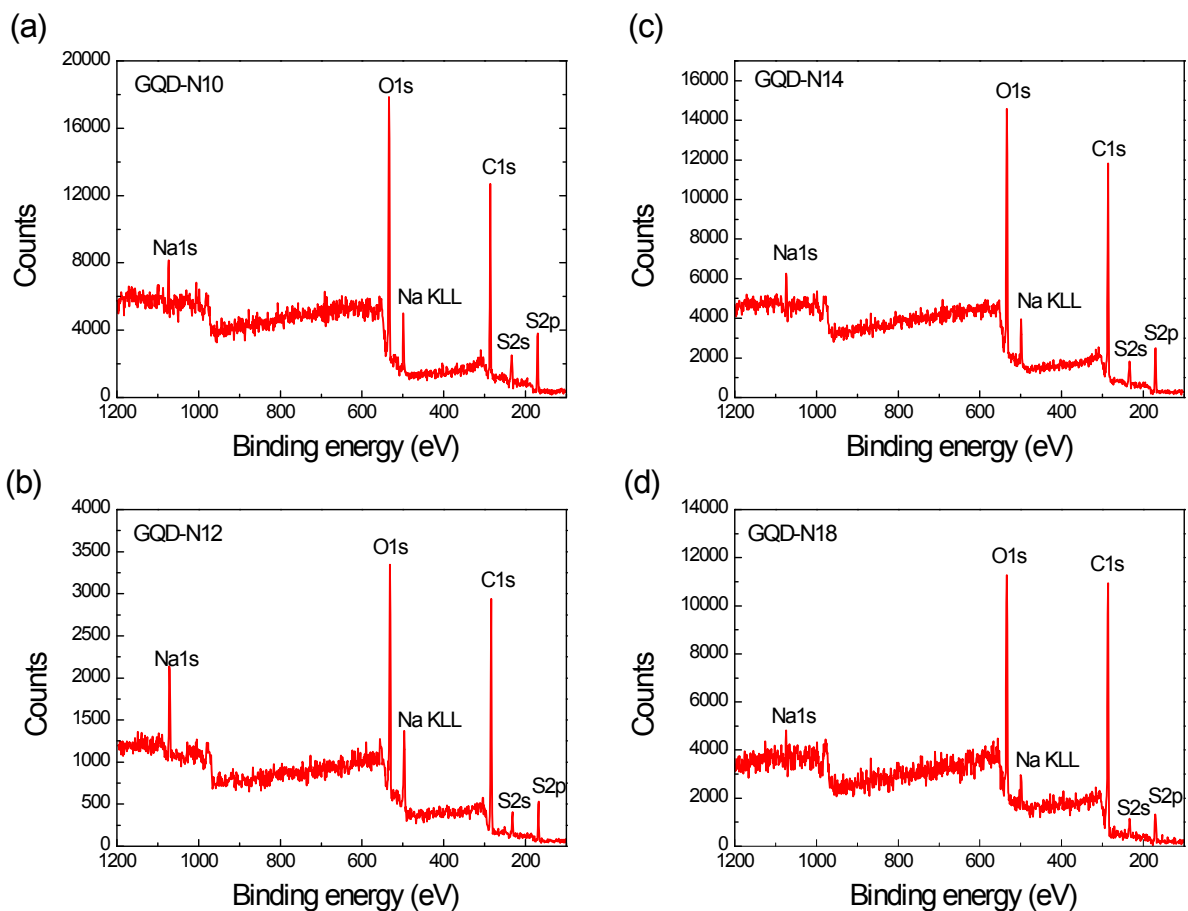


Figure S4. XPS survey scans of (a) GQD-N10, (b) GQD-N12, (c) GQD-N14 and (d) GQD-N18 samples.

Table S1. Summarized XPS data of GQD-N10, GQD-N12, GQD-N14 and GQD-N18 samples.

| Sample | C:O (at % : at %) |
|---------|-------------------|
| GQD-N10 | 2.40:1 |
| GQD-N12 | 2.44:1 |
| GQD-N14 | 2.47:1 |
| GQD-N18 | 2.54:1 |

S7. Gas chromatography-mass spectrometry (GC-MS) measurement

Gas chromatography-mass spectrometry (GC-MS) (Agilent 7890B/5977A) is performed to analyze the distribution of the fragments and moieties during the plasma-assisted synthesis. Plasma-treated samples were injected into column (DB-WAX, (30m length x 0.25mm inner diameter x 0.25um coating film thickness))

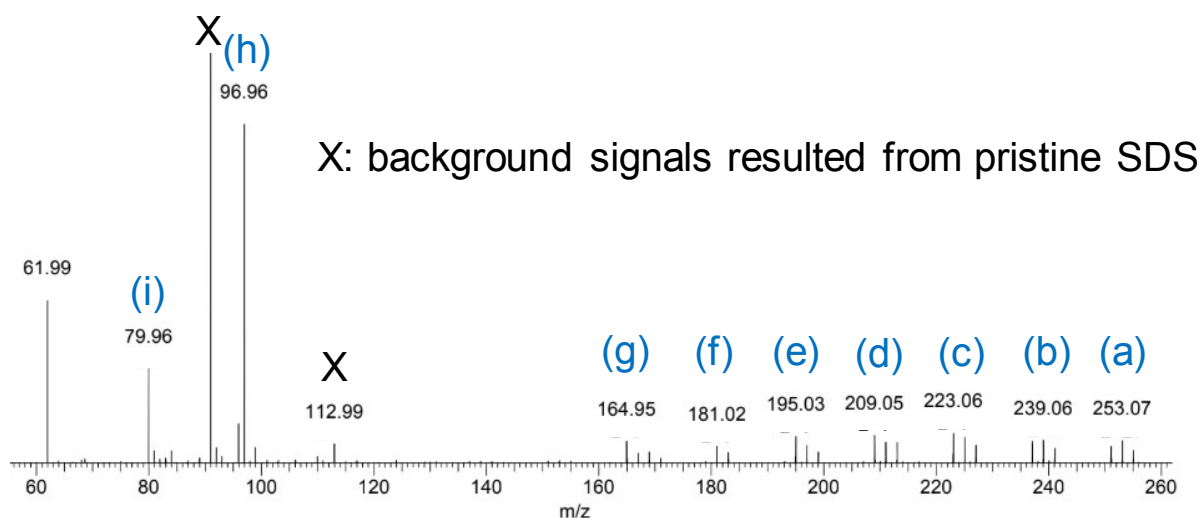
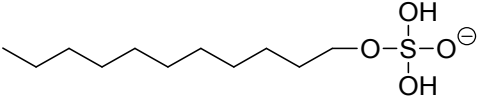
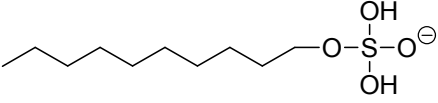
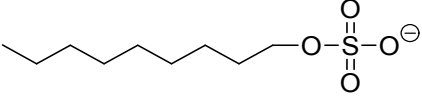
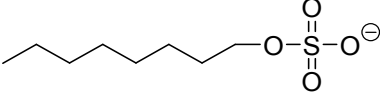
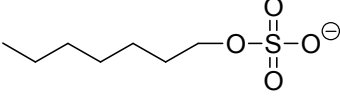
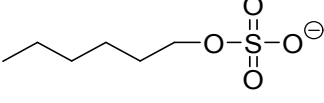
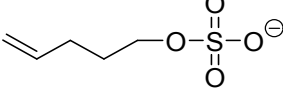
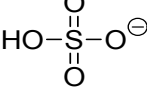
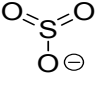


Figure S5. GC-MS spectra of 1 wt% SDS aqueous solution treated with microplasma for 1 hr at a constant discharge current of 9.6 mA .

Table S2. Summarized GC-MS data of 1 wt% SDS aqueous solution treated with a microplasma for 1 hr at a constant discharge current of 9.6 mA .

| label | proposed chemical structure | composition | calculated mass |
|----------------|---|----------------------|-----------------|
| a |  | $C_{11}H_{25}O_4S^-$ | 253 |
| b |  | $C_{10}H_{23}O_4S^-$ | 239 |
| c |  | $C_9H_{19}O_4S^-$ | 223 |
| d |  | $C_8H_{17}O_4S^-$ | 209 |
| e |  | $C_7H_{15}O_4S^-$ | 195 |
| f |  | $C_6H_{13}O_4S^-$ | 181 |
| g ^a |  | $C_5H_9O_4S^-$ | 165 |
| h |  | HO_4S^- | 97 |
| i |  | O_3S^- | 80 |

a The exact position of olefin functionality is not determined.

S8. DFT calculation

Quantum-chemical calculations were performed with the Gaussian09 suite employing the WB97XD density functional in combination with the 6-311G(d,p) basis set. Geometry optimizations were performed with solvation in water by applying the SMD model and the GEDIIS optimization algorithm. The minimum nature of each stationary point was confirmed by frequency analysis. One tiny imaginary frequency (-7.96 cm^{-1}) was found for SDS(0,1), which should be an artifact and have a negligible effect on the final results.

Cartesian coordinates (Å) of the optimized structures:

SDS(0,1)

| | | | |
|---|-----------------|----------------|-----------------|
| C | -1.285056812847 | 1.105726817079 | -0.069037970421 |
| H | -0.900133332411 | 0.081112082368 | -0.093773337761 |
| H | -0.936908012348 | 1.615030362230 | -0.972087880997 |
| H | -2.377435764672 | 1.051226724934 | -0.117025782523 |
| C | -0.829173676177 | 1.830004424086 | 1.193201999034 |
| H | -1.201789386456 | 2.861153973266 | 1.179274465270 |
| H | 0.265209341879 | 1.896545734353 | 1.203565578903 |
| C | -1.299875067500 | 1.145039729344 | 2.473969772555 |
| H | -0.929299164307 | 0.111793760897 | 2.487344994844 |
| H | -2.395625959981 | 1.080302980022 | 2.465914442446 |
| C | -0.845489111426 | 1.859473650450 | 3.743513110358 |
| H | -1.215886437531 | 2.892638099223 | 3.728902909774 |
| H | 0.250186513301 | 1.923983446561 | 3.749258744700 |
| C | -1.313947849022 | 1.175715599369 | 5.025205606748 |
| H | -0.946771595490 | 0.141408136987 | 5.038593275375 |
| H | -2.409803474707 | 1.115262105760 | 5.023261387041 |
| C | -0.850446377206 | 1.890086928403 | 6.291623706588 |
| H | -1.216845216161 | 2.924664021580 | 6.277132556220 |
| H | 0.245454753385 | 1.950359226449 | 6.291487849831 |
| C | -1.314615255753 | 1.211086714030 | 7.577310085442 |
| H | -0.950681118408 | 0.175691779660 | 7.592061621580 |
| H | -2.410614091869 | 1.154574872340 | 7.581784582712 |
| C | -0.841230656552 | 1.928875725771 | 8.838074627710 |
| H | -1.203844454716 | 2.964649803432 | 8.821307127652 |
| H | 0.254785747719 | 1.984574105273 | 8.832025178024 |

| | | | |
|----|-----------------|----------------|-----------------|
| C | -1.301621336321 | 1.257219138985 | 10.128600828824 |
| H | -0.939292071265 | 0.221752285661 | 10.149417925787 |
| H | -2.397381625337 | 1.204442073647 | 10.140181876595 |
| C | -0.818660752066 | 1.984861990163 | 11.379822497127 |
| H | -1.179983684831 | 3.020140254571 | 11.357686820988 |
| H | 0.276774796898 | 2.035278759056 | 11.369513878253 |
| C | -1.281647297696 | 1.315421030071 | 12.671621252308 |
| H | -0.912913262947 | 0.285311659135 | 12.711162267398 |
| H | -2.375360821648 | 1.277709918156 | 12.700006024903 |
| C | -0.779859991145 | 2.068028203952 | 13.882163726513 |
| H | -1.161739111173 | 3.092140816337 | 13.896781296364 |
| H | 0.312692092926 | 2.087085142875 | 13.910632906307 |
| O | -1.262612878770 | 1.373559689748 | 15.062080556691 |
| S | -0.829031876794 | 1.976684328512 | 16.492455261248 |
| O | -1.347710700742 | 3.336798576634 | 16.566516078493 |
| O | 0.645920932896 | 1.892174805556 | 16.560501601882 |
| O | -1.437497610472 | 1.017818993044 | 17.429573689361 |
| Na | 0.675413297741 | 0.143994390035 | 18.186536649851 |

SDS(-1,2)

| | | | |
|---|-----------------|----------------|-----------------|
| C | -1.361653403760 | 1.147833651549 | -0.072824213156 |
| H | -0.990388294389 | 0.119040157990 | -0.121015756584 |
| H | -1.030740185090 | 1.664433003142 | -0.978201422567 |
| H | -2.455469661465 | 1.107511091164 | -0.092375272789 |
| C | -0.863667966974 | 1.849902636508 | 1.186144610465 |
| H | -1.220696575587 | 2.886635224623 | 1.193307884682 |
| H | 0.231486849028 | 1.899544809490 | 1.170550819481 |
| C | -1.315397554331 | 1.157302748599 | 2.469658423764 |
| H | -0.957317161236 | 0.119580629035 | 2.464605634861 |
| H | -2.411750924740 | 1.106006419193 | 2.484158555054 |
| C | -0.826961463210 | 1.853105961134 | 3.736976311282 |
| H | -1.182644433871 | 2.891562724575 | 3.738175969881 |
| H | 0.269405727194 | 1.901596326640 | 3.723880049774 |
| C | -1.284840687614 | 1.164829047528 | 5.020101139635 |
| H | -0.925460741845 | 0.127714761099 | 5.022822916609 |
| H | -2.381070054751 | 1.112718947359 | 5.030516659532 |
| C | -0.803092531158 | 1.868036941523 | 6.286000349485 |
| H | -1.160310604741 | 2.905931461637 | 6.279690945544 |

| | | | |
|----|-----------------|----------------|-----------------|
| H | 0.293232380331 | 1.918233055944 | 6.277472707936 |
| C | -1.265285870751 | 1.186932479436 | 7.571329032050 |
| H | -0.902954962918 | 0.150968175022 | 7.583405577837 |
| H | -2.361386574563 | 1.132037166336 | 7.577181978854 |
| C | -0.790872759863 | 1.901612246953 | 8.833487064792 |
| H | -1.150826530205 | 2.938350218897 | 8.817205799096 |
| H | 0.305275032014 | 1.954362805551 | 8.829668573790 |
| C | -1.257140993888 | 1.229890385368 | 10.121934129305 |
| H | -0.891498254454 | 0.195712319680 | 10.146738234654 |
| H | -2.352826182837 | 1.173230591813 | 10.125450089333 |
| C | -0.787398106744 | 1.960931026777 | 11.376196747928 |
| H | -1.150299006185 | 2.995561737110 | 11.347662516305 |
| H | 0.308005636074 | 2.013423988994 | 11.377105405498 |
| C | -1.263435781697 | 1.294556636568 | 12.664774483436 |
| H | -0.890536193163 | 0.266339969990 | 12.713662672048 |
| H | -2.357360584956 | 1.251086681689 | 12.678002536249 |
| C | -0.784007926699 | 2.054848471596 | 13.880082681903 |
| H | -1.166565672716 | 3.079193541838 | 13.877879573549 |
| H | 0.308091800781 | 2.077116371860 | 13.926217277863 |
| O | -1.286610712304 | 1.370667369332 | 15.054194906243 |
| S | -0.900440254802 | 2.007602041309 | 16.490934772626 |
| O | -1.447813164479 | 3.362106368379 | 16.517035417525 |
| O | 0.570491334969 | 1.960155947931 | 16.591522227684 |
| O | -1.531046725299 | 1.063978653828 | 17.423490018827 |
| Na | 0.649431382891 | 0.239218065012 | 18.413335759716 |

SDS(-2,1)

| | | | |
|---|------------------|-----------------|-----------------|
| C | -10.692260759448 | -0.541950949089 | 0.043876979798 |
| H | -10.661566388216 | -1.633104096905 | -0.039568238835 |
| H | -11.577206532532 | -0.189874006215 | -0.493625240938 |
| H | -10.823510979358 | -0.293406004536 | 1.102014084261 |
| C | -9.415883991876 | 0.083645604562 | -0.508692387863 |
| H | -9.482791703626 | 1.175897000906 | -0.439567429602 |
| H | -9.323552187906 | -0.153334914069 | -1.575322546486 |
| C | -8.158619624667 | -0.389016463982 | 0.217168366846 |
| H | -8.095311527830 | -1.483120549795 | 0.154234316557 |
| H | -8.245208096368 | -0.145615577741 | 1.284143086505 |
| C | -6.875613453302 | 0.221814069456 | -0.338960443574 |

| | | | |
|----|-----------------|-----------------|-----------------|
| H | -6.937771759498 | 1.315749904055 | -0.274066829717 |
| H | -6.795979438528 | -0.019707050634 | -1.406831781136 |
| C | -5.613596560945 | -0.254750081833 | 0.375142020535 |
| H | -5.560915612907 | -1.349929856704 | 0.324835782273 |
| H | -5.679492601131 | 0.003404872073 | 1.439918092485 |
| C | -4.335162581168 | 0.336244320036 | -0.212393623458 |
| H | -4.385128202976 | 1.431478178952 | -0.160564013268 |
| H | -4.279578189658 | 0.080488223818 | -1.278447830649 |
| C | -3.062538771733 | -0.143738938314 | 0.480173951193 |
| H | -3.025786892442 | -1.240293338885 | 0.449827282892 |
| H | -3.096641729819 | 0.136232372869 | 1.540752508062 |
| C | -1.793493932420 | 0.418060773610 | -0.154570932259 |
| H | -1.825209734500 | 1.514566782377 | -0.119261750087 |
| H | -1.773960618678 | 0.144111162549 | -1.217182267432 |
| C | -0.508121035092 | -0.070489004587 | 0.507060021989 |
| H | -0.485023545943 | -1.167365841276 | 0.488122420209 |
| H | -0.504720453807 | 0.223318893694 | 1.563979456160 |
| C | 0.745700658633 | 0.469266036576 | -0.175098929154 |
| H | 0.733881891210 | 1.565550068323 | -0.141103971225 |
| H | 0.725237463944 | 0.190018588988 | -1.235488867269 |
| C | 2.038825417452 | -0.044643636798 | 0.452706882543 |
| H | 2.062773181317 | -1.138603722941 | 0.407602777179 |
| H | 2.085212320857 | 0.243277688117 | 1.507915362498 |
| C | 3.249387985549 | 0.504619824182 | -0.268817574235 |
| H | 3.299114654322 | 1.593623028632 | -0.173908212765 |
| H | 3.226031945836 | 0.238767279479 | -1.329010319610 |
| O | 4.427419367086 | -0.078756041873 | 0.330967404754 |
| S | 5.864926852432 | 0.495489611665 | -0.175815100628 |
| O | 5.942076875141 | 1.883834056525 | 0.288198295143 |
| O | 5.869465351572 | 0.365761523600 | -1.637287193602 |
| O | 6.794309046857 | -0.415177041587 | 0.503976836394 |
| Na | 8.213375032610 | -1.942771583289 | -0.873024234569 |

SDS(-3,2)

| | | | |
|---|-----------------|-----------------|-----------------|
| C | 10.944075788280 | 0.108243538302 | 0.172535852512 |
| H | 10.998964864793 | -0.401508819817 | 1.139823105328 |
| H | 11.790116183495 | 0.798350969826 | 0.110555262624 |
| H | 11.070589887206 | -0.648053626481 | -0.608909231117 |

| | | | |
|---|-----------------|-----------------|-----------------|
| C | 9.615098165495 | 0.839496604715 | 0.015078957394 |
| H | 9.599444624592 | 1.368869898858 | -0.945042592652 |
| H | 9.524970450585 | 1.607463678657 | 0.792509906743 |
| C | 8.408329366840 | -0.092506845097 | 0.091000701306 |
| H | 8.424971719478 | -0.626058189288 | 1.050250051099 |
| H | 8.494311901657 | -0.859173710739 | -0.689939308698 |
| C | 7.074350035301 | 0.633311340227 | -0.058332243761 |
| H | 7.058666299390 | 1.167213437759 | -1.017254997878 |
| H | 6.991550733020 | 1.399934140609 | 0.722843974175 |
| C | 5.865347224187 | -0.294872473478 | 0.019613189767 |
| H | 5.885330133247 | -0.834106127709 | 0.975474657454 |
| H | 5.941611039933 | -1.056961863589 | -0.766545674141 |
| C | 4.533442626091 | 0.437802909175 | -0.115217044952 |
| H | 4.511090203074 | 0.975131435001 | -1.072065945433 |
| H | 4.461597652335 | 1.201951030254 | 0.669399113846 |
| C | 3.321083630013 | -0.485143352484 | -0.028317867051 |
| H | 3.349761693604 | -1.029195509258 | 0.924579610061 |
| H | 3.384157459353 | -1.243482125862 | -0.819156384847 |
| C | 1.991455940087 | 0.254983541353 | -0.142836743626 |
| H | 1.957210036744 | 0.793514239300 | -1.098552171392 |
| H | 1.934865548481 | 1.017978400694 | 0.643974380671 |
| C | 0.776812981121 | -0.662792325831 | -0.038330511534 |
| H | 0.816537189629 | -1.207124690913 | 0.913675680084 |
| H | 0.822269875352 | -1.419925314234 | -0.831037303721 |
| C | -0.548706800913 | 0.087229406262 | -0.131067456521 |
| H | -0.599385823044 | 0.619337576997 | -1.088828919675 |
| H | -0.586155707092 | 0.852629409451 | 0.653525173815 |
| C | -1.760563991982 | -0.831175361009 | 0.003692638479 |
| H | -1.719165643375 | -1.357861641663 | 0.963068806765 |
| H | -1.745598392101 | -1.587855054355 | -0.787582446005 |
| C | -3.055647483892 | -0.053463137836 | -0.074572543001 |
| H | -3.158931283252 | 0.437267407444 | -1.047160056527 |
| H | -3.101456806589 | 0.704661231993 | 0.712931930570 |
| O | -4.141558310598 | -0.984036475872 | 0.103081093992 |
| S | -5.655391977953 | -0.363321133420 | 0.037367268357 |
| O | -5.801098965598 | 0.190723290950 | -1.313403670321 |
| O | -5.716395784656 | 0.651393747800 | 1.095231737677 |
| O | -6.459506164380 | -1.557725744437 | 0.293686848316 |

Na -11.117114034458 1.559046117281 0.072051634625

SDS(-4,1)

| | | | |
|---|------------------|-----------------|-----------------|
| C | -10.433630357797 | -1.069506011855 | 0.199167089528 |
| H | -10.334740137184 | -2.109788375098 | 0.525194842551 |
| H | -11.330519149232 | -0.997130818414 | -0.422376608941 |
| H | -10.595361969389 | -0.455983053917 | 1.091441031255 |
| C | -9.189625284422 | -0.614112432237 | -0.556866908201 |
| H | -9.320367968611 | 0.422618885115 | -0.888926472773 |
| H | -9.071065473910 | -1.216844716372 | -1.465107662873 |
| C | -7.916487009905 | -0.716858375893 | 0.279642586028 |
| H | -7.782680605633 | -1.756179225015 | 0.606073167892 |
| H | -8.036631874549 | -0.119959503749 | 1.193344735149 |
| C | -6.664145422311 | -0.256334946013 | -0.461052258497 |
| H | -6.794664460387 | 0.785808533090 | -0.780173411493 |
| H | -6.548126188522 | -0.848190935439 | -1.378438744398 |
| C | -5.390988993556 | -0.374694845387 | 0.372502412686 |
| H | -5.252713442337 | -1.422257556751 | 0.672182743923 |
| H | -5.508918545225 | 0.199187446020 | 1.300975346118 |
| C | -4.140950373305 | 0.099929559179 | -0.362328340786 |
| H | -4.264171024949 | 1.148618359590 | -0.661703446732 |
| H | -4.028725259586 | -0.482485592421 | -1.289968867408 |
| C | -2.863595173213 | -0.064303493398 | 0.453888645933 |
| H | -2.721602523416 | -1.140208700322 | 0.653069317073 |
| H | -2.964806149762 | 0.435269940875 | 1.425540311949 |
| C | -1.622394845453 | 0.436967236323 | -0.274242053328 |
| H | -1.742292103140 | 1.491894601915 | -0.551324998220 |
| H | -1.530474222681 | -0.136728707283 | -1.211739312752 |
| C | -0.340886127602 | 0.244527851837 | 0.529242410889 |
| H | -0.218540385121 | -0.830283862103 | 0.729123973148 |
| H | -0.431082293851 | 0.737714346189 | 1.505147037246 |
| C | 0.900594833778 | 0.759564632947 | -0.192651639002 |
| H | 0.797900872905 | 1.836616952520 | -0.373912511220 |
| H | 0.966950622988 | 0.281382539551 | -1.178045237471 |
| C | 2.188192348245 | 0.492697022756 | 0.583087588556 |
| H | 2.310694157085 | -0.585828396164 | 0.729623701314 |
| H | 2.130745603047 | 0.955023287700 | 1.574123243978 |
| C | 3.398029397647 | 1.030661543829 | -0.147814255043 |

| | | | |
|----|-----------------|-----------------|-----------------|
| H | 3.340196996172 | 2.118131801380 | -0.253431885270 |
| H | 3.487373609982 | 0.579074601514 | -1.139969061518 |
| O | 4.567350876933 | 0.694785523396 | 0.629017066698 |
| S | 6.002753369629 | 1.214126424932 | 0.055010005916 |
| O | 5.931545229256 | 2.680249840932 | 0.045920410638 |
| O | 6.141183109797 | 0.633679567256 | -1.285735567073 |
| O | 6.926720888541 | 0.664245380227 | 1.046969197530 |
| Na | -1.683362158547 | -4.625414492441 | -2.034939507871 |

SDS(-5,2)

| | | | |
|---|-----------------|-----------------|-----------------|
| C | 9.424951554690 | 1.347134817566 | 0.224821056037 |
| H | 9.070228973018 | 2.167004048999 | 0.857688751788 |
| H | 10.208391162080 | 1.743062460402 | -0.427439744192 |
| H | 9.880532319105 | 0.595643977675 | 0.877944098071 |
| C | 8.276537988244 | 0.747899690863 | -0.580802366582 |
| H | 8.658516729727 | -0.043970697883 | -1.236281175812 |
| H | 7.851980315481 | 1.517542642392 | -1.237523672614 |
| C | 7.162284835656 | 0.185013346918 | 0.297932528864 |
| H | 6.793542637430 | 0.983447446122 | 0.957873585502 |
| H | 7.568452546787 | -0.597365863707 | 0.952608821988 |
| C | 5.985923878132 | -0.365159381302 | -0.503163078258 |
| H | 6.323594737546 | -1.184989360468 | -1.151065300425 |
| H | 5.617668923465 | 0.431726740043 | -1.166367554722 |
| C | 4.821685389227 | -0.827405567403 | 0.369420278733 |
| H | 4.565494901075 | -0.010262287714 | 1.061047720063 |
| H | 5.126821080461 | -1.677256280384 | 0.993921399629 |
| C | 3.570642312277 | -1.174499642009 | -0.435598342333 |
| H | 3.733623628297 | -2.086246144529 | -1.025655111940 |
| H | 3.395858324708 | -0.359223991960 | -1.153569655440 |
| C | 2.318375542764 | -1.312336684777 | 0.429069698367 |
| H | 2.290927706681 | -0.463004015928 | 1.129211675394 |
| H | 2.370981052259 | -2.220034042735 | 1.044539538323 |
| C | 1.026368399366 | -1.290109880408 | -0.383323763408 |
| H | 0.984562087436 | -2.153106618633 | -1.060800306835 |
| H | 1.045060721327 | -0.390383931807 | -1.016949997422 |
| C | -0.231044363818 | -1.243225661307 | 0.480860759748 |
| H | -0.106266183926 | -0.458268678705 | 1.240416010524 |
| H | -0.351666304309 | -2.189281358111 | 1.023715365826 |

| | | | |
|----|-----------------|-----------------|-----------------|
| C | -1.489357685682 | -0.942126701501 | -0.327870248295 |
| H | -1.604595823892 | -1.686321812035 | -1.125626987475 |
| H | -1.360749482005 | 0.029752954919 | -0.822094685487 |
| C | -2.754995878801 | -0.908576459605 | 0.524921699243 |
| H | -2.627768430265 | -0.197644352066 | 1.348452946248 |
| H | -2.935131704249 | -1.895013864677 | 0.965460297988 |
| C | -3.957664300402 | -0.501325008007 | -0.296823065350 |
| H | -4.117656605543 | -1.191700696013 | -1.130136166619 |
| H | -3.828979902531 | 0.510951776819 | -0.691006771970 |
| O | -5.117024417435 | -0.530485169505 | 0.563157934660 |
| S | -6.495212768605 | 0.087927017743 | -0.050303829398 |
| O | -6.772397544324 | -0.670042872266 | -1.276674181755 |
| O | -6.227359941481 | 1.509639551448 | -0.298049593288 |
| O | -7.438551518475 | -0.163776729932 | 1.038604971643 |
| Na | 2.698188522640 | 3.004551298852 | 0.609617071629 |

SDS(-6,1)

| | | | |
|---|----------------|-----------------|-----------------|
| C | 8.540143301759 | 2.174242812033 | 0.219117717676 |
| H | 7.954858645738 | 2.873112485800 | 0.825673241787 |
| H | 9.198796038113 | 2.761754176042 | -0.426815448114 |
| H | 9.170652460305 | 1.591412178972 | 0.898653584565 |
| C | 7.624375604254 | 1.262385356416 | -0.591774010979 |
| H | 8.227183779509 | 0.600350312397 | -1.225108681481 |
| H | 7.010518873159 | 1.870010526340 | -1.269248693416 |
| C | 6.697962300306 | 0.425663023305 | 0.286080248788 |
| H | 6.073811099637 | 1.107799269736 | 0.886901048195 |
| H | 7.291940913325 | -0.169350783902 | 0.992367074294 |
| C | 5.761873078863 | -0.477202338144 | -0.511076867878 |
| H | 6.334575741835 | -1.155760640912 | -1.156294662241 |
| H | 5.160545483045 | 0.168914519778 | -1.171237272827 |
| C | 4.797711042253 | -1.255931781451 | 0.382764225127 |
| H | 4.389190684790 | -0.542239898938 | 1.113287852475 |
| H | 5.336021134360 | -2.018447380953 | 0.959853398374 |
| C | 3.622212840345 | -1.871333741749 | -0.381837233445 |
| H | 3.934028774878 | -2.778211147832 | -0.915403193665 |
| H | 3.311820782235 | -1.147625703495 | -1.149160971585 |
| C | 2.404226026527 | -2.145493132660 | 0.503547163911 |
| H | 2.289102166330 | -1.284426808832 | 1.177640959438 |

| | | | |
|----|-----------------|-----------------|-----------------|
| H | 2.573705594664 | -3.020188315836 | 1.144660845200 |
| C | 1.099311314990 | -2.288310360136 | -0.284293142348 |
| H | 1.041865742503 | -3.268284047427 | -0.774671220832 |
| H | 1.115510264196 | -1.539603048604 | -1.088402454567 |
| C | -0.149828225788 | -2.025742655194 | 0.562566853210 |
| H | 0.088050501287 | -1.213900533430 | 1.264650192787 |
| H | -0.409074089366 | -2.901564167662 | 1.170151263001 |
| C | -1.346086581707 | -1.566781043631 | -0.272258138427 |
| H | -1.755016659537 | -2.392364168311 | -0.866870138101 |
| H | -0.977898587199 | -0.813993811797 | -0.984449797927 |
| C | -2.444682599737 | -0.911099575031 | 0.565828997285 |
| H | -1.975774819512 | -0.230893738464 | 1.291071752181 |
| H | -3.023678010441 | -1.655581572172 | 1.121986342861 |
| C | -3.352843645783 | -0.078558716009 | -0.310977081162 |
| H | -3.832317863455 | -0.676498504692 | -1.091629945278 |
| H | -2.761864246366 | 0.726373762457 | -0.771861303566 |
| O | -4.374150556272 | 0.504731523963 | 0.529337764811 |
| S | -5.260330992193 | 1.705593415502 | -0.122084802002 |
| O | -5.869093068660 | 1.146879025778 | -1.337037604175 |
| O | -4.333297095798 | 2.809928953256 | -0.397386052806 |
| O | -6.214497915946 | 1.978395678123 | 0.953748723339 |
| Na | 1.546844768554 | 2.239858597365 | 0.018198467518 |

SDS(-7,2)

| | | | |
|---|----------------|-----------------|-----------------|
| C | 7.545159244832 | 2.655871483452 | 0.187282584512 |
| H | 6.743403155129 | 3.123521938160 | 0.774257994887 |
| H | 7.963322012912 | 3.420303667659 | -0.474644958398 |
| H | 8.333144050601 | 2.340919323548 | 0.879575096696 |
| C | 6.986987463234 | 1.474396924313 | -0.600459570491 |
| H | 7.745234718873 | 1.070299732661 | -1.281986033844 |
| H | 6.151760341177 | 1.836767821744 | -1.222114703877 |
| C | 6.440994861374 | 0.373175384643 | 0.306236818149 |
| H | 5.699849813618 | 0.842099597645 | 0.973604248179 |
| H | 7.237110860879 | -0.031161585219 | 0.944744852375 |
| C | 5.729105533060 | -0.742769956058 | -0.459954886220 |
| H | 6.447436472251 | -1.360723091622 | -1.013391856995 |
| H | 5.082520747551 | -0.261318549873 | -1.207944229037 |
| C | 4.824562561197 | -1.596709089180 | 0.432848777018 |

| | | | |
|----|-----------------|-----------------|-----------------|
| H | 4.294395404855 | -0.900352146589 | 1.098589308142 |
| H | 5.415394304140 | -2.259973797509 | 1.076526976055 |
| C | 3.759528254817 | -2.379978505106 | -0.348672246919 |
| H | 4.175777085495 | -3.307779938625 | -0.757700465993 |
| H | 3.474045343877 | -1.765305071221 | -1.211428530559 |
| C | 2.482264182144 | -2.652672123091 | 0.467859761427 |
| H | 2.432096523469 | -1.903945663298 | 1.268847546355 |
| H | 2.520723535918 | -3.631880715085 | 0.958982211479 |
| C | 1.198128891104 | -2.500005088010 | -0.357401573959 |
| H | 1.022583417609 | -3.377569658744 | -0.991904582491 |
| H | 1.350217292544 | -1.645414844969 | -1.032944912162 |
| C | -0.031660315976 | -2.171425576202 | 0.491636408502 |
| H | 0.279607996759 | -1.418524700908 | 1.230916945539 |
| H | -0.382596198120 | -3.046902386382 | 1.051596073631 |
| C | -1.161552086217 | -1.549316676194 | -0.330999912980 |
| H | -1.657931591675 | -2.298737756895 | -0.958663645483 |
| H | -0.701741279554 | -0.815239812645 | -1.009112636531 |
| C | -2.179671739344 | -0.799927112887 | 0.529493113730 |
| H | -1.632138276974 | -0.178711168552 | 1.253642849925 |
| H | -2.820405193329 | -1.490109084659 | 1.088293526674 |
| C | -3.015429926866 | 0.136663622694 | -0.314450025467 |
| H | -3.607694146910 | -0.396120359540 | -1.064390022434 |
| H | -2.352118788256 | 0.861098995811 | -0.808713225634 |
| O | -3.907264874693 | 0.849592998924 | 0.573124159346 |
| S | -4.659499621752 | 2.161102237612 | -0.030470320436 |
| O | -5.450914183320 | 1.681711674800 | -1.172846025665 |
| O | -3.612346853313 | 3.114859228791 | -0.414527688548 |
| O | -5.463694633495 | 2.584165037501 | 1.118035851026 |
| Na | 1.817709640373 | 2.474042789104 | 0.126835950478 |

SDS(-8,1)

| | | | |
|---|----------------|----------------|-----------------|
| C | 6.843690894636 | 2.818303103120 | 0.274947694271 |
| H | 5.884324973224 | 3.294090273786 | 0.534871433438 |
| H | 7.417398493355 | 3.533712081740 | -0.322980927099 |
| H | 7.397263099472 | 2.629490133422 | 1.201399378928 |
| C | 6.572803995007 | 1.526561271441 | -0.492296015108 |
| H | 7.498979920977 | 1.118159289755 | -0.914721994788 |
| H | 5.904277103719 | 1.766528545094 | -1.337170052101 |

| | | | |
|----|-----------------|-----------------|-----------------|
| C | 5.866298427038 | 0.479294229291 | 0.367396241007 |
| H | 4.963530415650 | 0.956544596476 | 0.787905420725 |
| H | 6.498207912356 | 0.188299049451 | 1.216768181176 |
| C | 5.409031767321 | -0.755973436868 | -0.410175024403 |
| H | 6.267189882938 | -1.373518733555 | -0.706671689827 |
| H | 4.920156646058 | -0.410326190474 | -1.336706013233 |
| C | 4.380721365256 | -1.573487222633 | 0.367386238536 |
| H | 3.502268943127 | -0.920252124224 | 0.497128535089 |
| H | 4.752173985843 | -1.796536630243 | 1.376311659556 |
| C | 3.943052427841 | -2.878454393413 | -0.307057112429 |
| H | 4.700642532025 | -3.651314008243 | -0.131903398247 |
| H | 3.898643445934 | -2.732529183360 | -1.394309384234 |
| C | 2.567323437433 | -3.350139432626 | 0.185137643728 |
| H | 2.519806119570 | -3.200890222040 | 1.271704471260 |
| H | 2.457980224289 | -4.427634611369 | 0.023655171508 |
| C | 1.401050715556 | -2.600471078991 | -0.489631245138 |
| H | 0.964402558800 | -3.225786636641 | -1.277808912626 |
| H | 1.782981757012 | -1.695866754286 | -0.992340717877 |
| C | 0.305845271681 | -2.127289354102 | 0.465850198207 |
| H | 0.754714860446 | -1.379669280075 | 1.137745137164 |
| H | -0.052744384975 | -2.951187231393 | 1.095716782008 |
| C | -0.858063762551 | -1.460452680878 | -0.272739851287 |
| H | -1.493568247479 | -2.212791628829 | -0.754981774703 |
| H | -0.428968409806 | -0.834321866638 | -1.072058264382 |
| C | -1.677507509833 | -0.537085096702 | 0.627496912201 |
| H | -0.976111376907 | 0.182375217806 | 1.084085827312 |
| H | -2.176052376751 | -1.092806697783 | 1.429211268220 |
| C | -2.680584194528 | 0.269349453967 | -0.168169365688 |
| H | -3.444840686893 | -0.357004591773 | -0.638274958898 |
| H | -2.145507320286 | 0.847766917147 | -0.936547319629 |
| O | -3.321517325742 | 1.190889509506 | 0.745020441254 |
| S | -4.177933183716 | 2.414566319350 | 0.095774730139 |
| O | -5.229074287797 | 1.778128152138 | -0.713435419000 |
| O | -3.247127410417 | 3.222461634835 | -0.700424037236 |
| O | -4.677142090648 | 3.083618137516 | 1.299677138892 |
| Na | 1.728385391762 | 2.763669171297 | -0.946578026684 |

SDS(-9,2)

| | | | |
|---|-----------------|-----------------|-----------------|
| C | 6.032666666225 | 3.376378262635 | -0.023670015021 |
| H | 5.040323365015 | 3.682640262888 | 0.342643118363 |
| H | 6.381458382949 | 4.135220737506 | -0.737523810794 |
| H | 6.736846006962 | 3.387258115930 | 0.827551941405 |
| C | 6.017370652946 | 1.991865613650 | -0.646778235085 |
| H | 7.182251095331 | 1.679702594410 | -0.846215028873 |
| H | 5.492937111298 | 1.987766760686 | -1.608422825197 |
| C | 5.506051415182 | 0.914767302438 | 0.287515057837 |
| H | 4.702886716570 | 1.283577957874 | 0.943856816805 |
| H | 6.374355165116 | 0.638090006293 | 0.945302996877 |
| C | 5.039630316901 | -0.344423160936 | -0.441268655822 |
| H | 5.905722447163 | -0.812026507247 | -0.940080647937 |
| H | 4.331044943736 | -0.052012009722 | -1.232275994091 |
| C | 4.323829500047 | -1.336145139074 | 0.472852024264 |
| H | 3.417933595391 | -0.825799199553 | 0.842254867310 |
| H | 4.936022249794 | -1.542843437825 | 1.360226611546 |
| C | 3.931185151174 | -2.663037939707 | -0.200574139499 |
| H | 4.723106481892 | -3.403619150448 | -0.043669521416 |
| H | 3.863901643382 | -2.516779696525 | -1.286677925619 |
| C | 2.583102857302 | -3.202960325558 | 0.299709298825 |
| H | 2.510405208075 | -3.023652604024 | 1.380294732862 |
| H | 2.527815513332 | -4.289468431380 | 0.166429404108 |
| C | 1.396989060100 | -2.538724950542 | -0.412450694185 |
| H | 1.214378986405 | -3.049904742492 | -1.366499430791 |
| H | 1.660424491005 | -1.497731945491 | -0.665142366797 |
| C | 0.112448645156 | -2.466456005226 | 0.409872564802 |
| H | 0.303164240318 | -1.769283209448 | 1.244178955988 |
| H | -0.141991634229 | -3.441186820292 | 0.845387676250 |
| C | -1.055247888871 | -1.906229503924 | -0.404659208361 |
| H | -1.407221679007 | -2.643075554560 | -1.136970478088 |
| H | -0.674309053501 | -1.042531684920 | -0.974329279417 |
| C | -2.209266428750 | -1.401592261022 | 0.462534077924 |
| H | -1.787443515398 | -0.731946582998 | 1.229237147945 |
| H | -2.726886406547 | -2.224065496330 | 0.967552323325 |
| C | -3.177471794954 | -0.571825139041 | -0.353223795527 |
| H | -3.691699263729 | -1.158865073522 | -1.120454015443 |
| H | -2.623748334588 | 0.256163259017 | -0.820751945295 |
| O | -4.157248177215 | -0.014673446823 | 0.553746390788 |

| | | | |
|----|-----------------|----------------|-----------------|
| S | -5.083505627251 | 1.202227453071 | -0.007632868572 |
| O | -5.855377470887 | 0.632309221429 | -1.123023812356 |
| O | -4.180036992379 | 2.281149580943 | -0.423575399764 |
| O | -5.890799659209 | 1.514347893496 | 1.174727708609 |
| Na | 0.774413741191 | 2.611524784917 | 0.557766602030 |

SDS(-10,1)

| | | | |
|---|-----------------|-----------------|-----------------|
| C | 6.669834538078 | 2.991717521485 | 0.039831703793 |
| H | 5.710950978258 | 3.274227117748 | 0.482305727659 |
| H | 7.228573030415 | 3.763939117638 | -0.484205533507 |
| H | 10.031633496862 | 3.260538897919 | -1.436802706572 |
| C | 7.126323055491 | 1.742497131448 | 0.110502982863 |
| H | 8.200725878334 | -2.687014148696 | 0.476411704483 |
| H | 8.070111138912 | 1.498285918647 | -0.379659468501 |
| C | 6.390092434419 | 0.608983189442 | 0.768488601456 |
| H | 5.613023270979 | 1.020291437386 | 1.428440740311 |
| H | 7.076336526707 | 0.017657753518 | 1.387741507186 |
| C | 5.701788172822 | -0.307873651500 | -0.252785455800 |
| H | 6.444579973358 | -0.802804890434 | -0.890883050384 |
| H | 5.083115088460 | 0.330376824223 | -0.901238436645 |
| C | 4.775151459244 | -1.323821940386 | 0.415286032157 |
| H | 4.171159089305 | -0.764956158797 | 1.147725096430 |
| H | 5.354754559844 | -2.070657585875 | 0.972735296114 |
| C | 3.799686579192 | -1.986130813762 | -0.565842225683 |
| H | 4.303164729121 | -2.757140830796 | -1.160869790269 |
| H | 3.480417626670 | -1.206188655999 | -1.269488741268 |
| C | 2.532722010317 | -2.533600548302 | 0.117792987993 |
| H | 2.385943057437 | -1.952918737994 | 1.038651432531 |
| H | 2.656945388320 | -3.579751558069 | 0.420794728583 |
| C | 1.259453944796 | -2.339755437363 | -0.718464150250 |
| H | 1.171301588215 | -3.093873634532 | -1.510168787055 |
| H | 1.354201186362 | -1.360091920981 | -1.211906390178 |
| C | -0.007934287931 | -2.261915020341 | 0.138375057524 |
| H | 0.238764499268 | -1.610302738210 | 0.991626492040 |
| H | -0.290960242575 | -3.241186627840 | 0.543186918020 |
| C | -1.177722868882 | -1.593332564140 | -0.588972031515 |
| H | -1.628190639114 | -2.260171698411 | -1.333453408960 |
| H | -0.764623519980 | -0.730909638593 | -1.133611097727 |

| | | | |
|----|-----------------|-----------------|-----------------|
| C | -2.233709712140 | -1.053998377453 | 0.379512039502 |
| H | -1.712396642064 | -0.535392259417 | 1.198580923266 |
| H | -2.836133509962 | -1.859801715515 | 0.811994445436 |
| C | -3.117514455555 | -0.022371489115 | -0.286832857692 |
| H | -3.717750100242 | -0.441656313578 | -1.099936228811 |
| H | -2.486566582829 | 0.792853833838 | -0.668513887788 |
| O | -4.002622428148 | 0.512107736273 | 0.726119860571 |
| S | -4.786485608186 | 1.895310876817 | 0.377807765218 |
| O | -5.606663382078 | 1.602133100236 | -0.807711700734 |
| O | -3.768287147573 | 2.923341575480 | 0.132478301376 |
| O | -5.563091582842 | 2.099546055560 | 1.603415195261 |
| Na | 1.386303408914 | 2.561828868441 | 0.759749409567 |

SDS-2H(-10,1)

| | | | |
|---|-----------------|-----------------|-----------------|
| C | 6.318355564304 | -3.200191730214 | -0.169087284915 |
| H | 5.450229703172 | -3.257135773794 | 0.553430526429 |
| H | 6.858306058528 | -4.158614086033 | 0.041785062993 |
| C | 7.273583572539 | -1.992502275644 | 0.068258202423 |
| H | 7.400212125288 | -1.768824098070 | 1.176837603231 |
| C | 6.630760026520 | -0.693514712645 | -0.462924040250 |
| H | 6.360363990455 | -0.865087110829 | -1.522328111956 |
| H | 7.347943626607 | 0.153987204818 | -0.474606795436 |
| C | 5.357549479337 | -0.175197292850 | 0.239272340374 |
| H | 5.622331124224 | 0.142977311032 | 1.259931548033 |
| H | 4.638645711673 | -1.003266970043 | 0.352885100459 |
| C | 4.619218476941 | 0.956136900398 | -0.482365739067 |
| H | 4.188672411267 | 0.537158413439 | -1.404503746189 |
| H | 5.322562679161 | 1.740516856720 | -0.796574297526 |
| C | 3.478877762596 | 1.551180761235 | 0.347743653666 |
| H | 3.876531419553 | 2.195963267954 | 1.142769045365 |
| H | 2.959198071184 | 0.712082723775 | 0.843076751241 |
| C | 2.418078147681 | 2.281887685751 | -0.478680198336 |
| H | 2.118524081814 | 1.585254269892 | -1.275963648241 |
| H | 2.836291606025 | 3.168194650986 | -0.971635529595 |
| C | 1.164620585488 | 2.630331209098 | 0.344251966802 |
| H | 1.268814242288 | 3.613756666739 | 0.818508690461 |
| H | 1.100909586167 | 1.901848424318 | 1.162374729809 |
| C | -0.144091567005 | 2.539734069453 | -0.455206218222 |

| | | | |
|----|-----------------|-----------------|-----------------|
| H | -0.032167009701 | 1.705366193740 | -1.163067918535 |
| H | -0.318227420801 | 3.446331090531 | -1.047504409565 |
| C | -1.355343056060 | 2.201307300026 | 0.418792430768 |
| H | -1.655933273627 | 3.049347353883 | 1.045382823858 |
| H | -1.036940681600 | 1.392273862705 | 1.093101173338 |
| C | -2.537880786921 | 1.665921354260 | -0.392645317640 |
| H | -2.151984976070 | 0.927478408663 | -1.113005586393 |
| H | -3.041537158525 | 2.460933698304 | -0.952703548026 |
| C | -3.519774814128 | 0.925441712408 | 0.490718356792 |
| H | -3.995539078044 | 1.574800156634 | 1.231664511679 |
| H | -2.989099067790 | 0.101968444370 | 0.993441329540 |
| O | -4.539093702951 | 0.361776096554 | -0.369036473329 |
| S | -5.472236385334 | -0.819067668778 | 0.252027015763 |
| O | -6.163541708456 | -0.217653827250 | 1.403217670314 |
| O | -4.584115148744 | -1.925568823634 | 0.627509896787 |
| O | -6.351547419697 | -1.112574001604 | -0.882896209168 |
| Na | 0.428677202640 | -2.494075716297 | -0.127083357736 |

SDS-2H(-12,1)

| | | | |
|---|-----------------|-----------------|-----------------|
| C | -5.050925953006 | 3.661295985285 | 0.891474225855 |
| H | -4.557113214080 | 3.281619808302 | 1.839282592014 |
| H | -5.767530819881 | 4.418610818678 | 1.298594650765 |
| C | -5.829343090336 | 2.562129358474 | 0.117132670103 |
| H | -6.359257559748 | 1.848093988341 | 0.831117585146 |
| C | -4.869962991361 | 1.607560979436 | -0.623479117578 |
| H | -4.245384312104 | 2.189813164015 | -1.333243251567 |
| H | -5.434586645355 | 0.888881067265 | -1.251535322040 |
| C | -3.877921735741 | 0.757351649614 | 0.207401130554 |
| H | -4.422876238739 | 0.300148102323 | 1.049425621030 |
| H | -3.110457858785 | 1.422206251202 | 0.644339133230 |
| C | -3.153030044648 | -0.324292492018 | -0.593909150279 |
| H | -2.518812566465 | 0.183443006465 | -1.343579166389 |
| H | -3.882567257563 | -0.925881840149 | -1.156103169879 |
| C | -2.261715910098 | -1.246932950609 | 0.240937906305 |
| H | -2.884589267994 | -1.852351262627 | 0.917385570598 |
| H | -1.623644499939 | -0.615456462600 | 0.883773347801 |
| C | -1.346043065476 | -2.152406490528 | -0.588625346142 |
| H | -0.644562505233 | -1.457949391572 | -1.101311186125 |

| | | | |
|----|-------------------|-----------------|-----------------|
| H | -1.955875046528 | -2.569206229614 | -1.413347664786 |
| C | -0.607259827602 | -3.262813141095 | 0.204686785243 |
| H | -115.513429357659 | -2.638795774501 | 0.469664289380 |
| H | -0.617668122409 | -2.919083481931 | 1.262537475417 |
| C | 0.886573501124 | -3.269685908402 | -0.190832189004 |
| H | 0.966095427121 | -3.172892717994 | -1.286804366698 |
| H | 1.376900231691 | -4.233617773516 | 0.032025924385 |
| C | 1.759760951636 | -2.162133701562 | 0.441418121581 |
| H | 1.970760929846 | -2.426381961206 | 1.487420037013 |
| H | 1.186382913863 | -1.221175202652 | 0.469856847494 |
| C | 3.060726247515 | -1.855700679485 | -0.302899481650 |
| H | 2.792969344861 | -1.365780716313 | -1.254584735696 |
| H | 3.625215648566 | -2.766930260031 | -0.532425490939 |
| C | 3.915404911608 | -0.877332324159 | 0.474337017616 |
| H | 4.352345979779 | -1.330876952966 | 1.370292947312 |
| H | 3.303995001431 | -0.002080448754 | 0.748704758717 |
| O | 4.978202116720 | -0.423116856156 | -0.401494171611 |
| S | 6.068169812815 | 0.620020865326 | 0.204764533220 |
| O | 6.944421384127 | -0.192510516555 | 1.066567886165 |
| O | 5.332579649994 | 1.647297138174 | 0.949908684587 |
| O | 6.730515576732 | 1.101897687756 | -1.009697512808 |
| Na | 0.853036048546 | 2.693191195537 | -1.150167934324 |

SDS-3H(-13,1)

| | | | |
|---|-----------------|-----------------|-----------------|
| C | -5.766566439185 | -3.106681910754 | -0.281070675849 |
| H | -5.828330865599 | -2.592761762878 | -1.289419497235 |
| H | -6.511866779503 | -3.932437844610 | -0.404204386234 |
| C | -6.184757746493 | -2.183907973298 | 0.897751520706 |
| H | -7.017965307734 | -1.470630385635 | 0.585578819102 |
| C | -5.053415199476 | -1.202062932388 | 1.268119870131 |
| H | -4.172760877601 | -1.764217455349 | 1.643261902996 |
| H | -5.362679562736 | -0.551918909624 | 2.110720059645 |
| C | -4.504904679922 | -0.266375167830 | 0.165237946673 |
| H | -5.352503169941 | 0.155627377343 | -0.399364659685 |
| H | -3.918959529763 | -0.873476753477 | -0.547038607116 |
| C | -3.610228657411 | 0.868484257827 | 0.663865652392 |
| H | -2.730893317259 | 0.423730649644 | 1.169068463206 |
| H | -4.144743235549 | 1.461767809014 | 1.420290094250 |

| | | | |
|----|-----------------|-----------------|-----------------|
| C | -3.099847047227 | 1.781694725758 | -0.450957446564 |
| H | -3.950109630257 | 2.227062369938 | -0.990290555814 |
| H | -2.557348641667 | 1.150059317531 | -1.178938384100 |
| C | -2.141377056789 | 2.884124212964 | 0.003052224483 |
| H | -1.239582501150 | 2.348256491613 | 0.381265167614 |
| H | -2.568741765306 | 3.363934641388 | 0.903170467869 |
| C | -1.828204430596 | 3.930332087182 | -1.087592021619 |
| H | -1.762858102287 | 3.350741517973 | -2.035879686784 |
| C | -0.406406586809 | 4.484059624141 | -0.864349431457 |
| H | -0.263052290272 | 4.692625589292 | 0.209309893266 |
| H | -0.246761381195 | 5.457148462091 | -1.359131598389 |
| C | 0.747403501945 | 3.550450820412 | -1.323559851536 |
| H | 0.720046623256 | 3.515825991714 | -2.422506705260 |
| H | 0.562949366199 | 2.523159848973 | -0.977436424187 |
| C | 2.113580724095 | 3.982927700149 | -0.880584330631 |
| H | 2.419438008783 | 4.989240694410 | -1.178308142007 |
| H | 2.271730242207 | 7.835671825925 | -1.602207880448 |
| C | 2.945160382250 | 3.246515697103 | -0.143856909104 |
| H | 3.917876239534 | 3.624234286410 | 0.163177377927 |
| H | 2.679958238704 | 2.233997839449 | 0.174991608687 |
| O | 4.596679845339 | -4.652687182733 | 1.306385316660 |
| S | 3.954945204750 | -5.952937820955 | 0.929916373039 |
| O | 4.867606228451 | -7.080364933390 | 1.338860963755 |
| O | 3.750851666578 | -6.014186975186 | -0.554131896396 |
| O | 2.642894901083 | -6.114630058609 | 1.634592738691 |
| Na | 0.693848736197 | -1.594344840652 | 0.05413775177 |

Reference

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