

Electronic Supplementary Information

Nanodiamonds in Sugar Rings: An Experimental and Theoretical Investigation of Cyclodextrin-Nanodiamond Inclusion Complexes

Jens Voskuhl,^a Mark Waller,^{a*} Sateesh Bandaru,^a Boryslav A. Tkachenko,^b Carlo Fregonese,^a Birgit Wibbeling,^a Peter R. Schreiner^{b*} and Bart Jan Ravoo^{a*}

a) *Organisch Chemisches Institut, Westfälische Wilhelms-Universität Münster, Corrensstrasse 40, 48149 Münster, Germany*

b) *Institut für Organische Chemie, Justus-Liebig University Heinrich-Buff-Ring 58, 35392 Giessen, Germany*

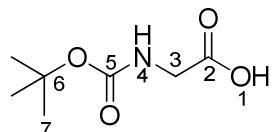
E-Mail: b.j.ravoo@uni-muenster.de, m.waller@uni-muenster.de, prs@org.chemie.uni-giessen.de

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1. General experimental procedures

Chemicals were purchased from Sigma Aldrich or from Acros Organics and used without further purification. Methanol and dimethylformamide (DMF) were dried by storage over molecular sieves (3 Å) for more than 3 days. Reactions were monitored by thin-layer chromatography (TLC), which was performed on 0.2 mm Merck precoated silica gel 60 F254 aluminum sheets. Spots were visualized by treatment with basic KMnO₄ solution. Column chromatography was carried out on silica gel 60 (0.063-0.2 mm, Merck). NMR spectra were recorded on Bruker spectrometers (AV300, AV400). Chemical shifts are given in units of parts per million (ppm) and expressed relative to the signals of deuterated solvents. Coupling constants (*J*) are reported in Hertz (Hz). Mass spectra were recorded with a MicroToF spectrometer (Bruker). Isothermal titration calorimetry (ITC) was performed by using a Nano-Isothermal Titration calorimeter III (model CSC 5300; Calorimetry Sciences Corporation, London, Utah, USA). ITC measurements were performed in milli-Q water. To solubilize the compounds NaOMe was added (3 eq. for the substituted nanodiamonds and 1.5 eq. for the non modified nanodiamonds).

2-(tert-butoxycarbonyl)amino acetic acid (2)



To a stirred solution of NaOH (2 g, 50 mmol) in 30 mL of *tert*-butanol and 45 mL of water, glycine (3 g, 40 mmol) was added stepwise. Within 30 minutes di-*tert*-butyldicarbonate (8.7 g, 40 mmol) was added and the resulting clear solution was stirred over night. After that time the solution was acidified with potassium hydrogen sulfate to pH 3 and extracted 3 times with 25 mL of EtOAc. The combined organic layers were dried over MgSO₄. The solvent was removed in vacuo and the product was obtained.

Yield: 6.9 g (39.5 mmol, 99%)

Empirical formula: C₇H₁₃NO₃ (colorless solid)

¹H-NMR (400 MHz, CDCl₃, 298 K): δ = 1.20 (s, 9H, 7-H), 3.81 (dd, *J*=5.45 Hz, 2H, 3-H), 5.43 (t, *J*=5.45 Hz, 1H, 4-H), 6.91 (s, 1H, 1-H).

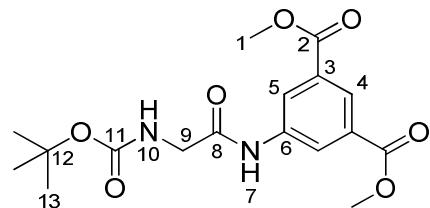
¹³C-NMR (101 MHz, CDCl₃, 298 K): δ = 30.74 (CH₃, 7-C), 42.16 (CH₂, 3-C), 70.02 (C_q, 6-C), 156.10 (C_q, 5-C), 173.33 (C_q, 2-C).

IR (neat): 735 (w), 779 (w), 856 (m), 958 (m), 1055 (m), 1158 (s), 1195 (s), 1255 (w), 1367 (m), 1409 (m), 1453 (w), 1531 (s), 1671 (s), 1736 (s), 2973 (w), 3342 (w).

HRMS-ESI (m/z): Calculated for $[C_7H_{13}NO_3Na]^+$: 198.0737, found 198.0731

Melting point: 78.5°C (EtOAc)

2-(tert-butoxycarbonyl)amino)acetamido-isophthalic acid dimethylester (3)



To a stirred solution of Boc-Gly-OH (1 g, 5.7 mmol) in 20 mL of DMF were added EDCI (1.2 g, 6.3 mmol) and HOBr (0.96 g, 6.3 mmol). After ten minutes 5-amino-isophthalate-dimethylester (1.2 g, 5.7 mmol), and NMM (0.7 mL, 6.3 mmol) were added. After stirring over night at room temperature the solvent was removed in vacuo. The residue was dissolved in $CHCl_3$ and extracted three times with water, saturated $NaHCO_3$ and brine. The organic layer was dried over $MgSO_4$ and the residue was applied to column chromatography on silica gel (pentane/EtOAc : 2:1, R_f = 0.32).

Yield: 1.03 g (2.9 mmol, 52 %)

Empirical formula: $C_{17}H_{22}N_2O_7$ (colorless solid)

¹H-NMR (400 MHz, CDCl₃, 298 K): δ = 1.38 (s, 9H, 13-H), 3.82 (s, 6H, 1-H), 3.98 (d, 2H, 9-H), 5.73 (t, 1H, 10-H), 8.27 (t, 1H, 4-H), 8.33 (d, 2H, 5-H), 9.44 (s, 1H, 7-H).

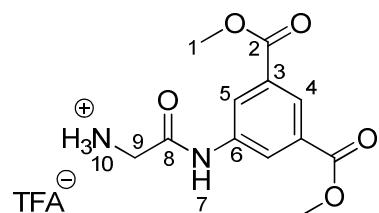
¹³C-NMR (101 MHz, CDCl₃, 298 K): δ = 27.29 (CH_3 , 13-C), 48.48 (CH_2 , 9-C), 51.41 (CH_3 , 1-C), 74.14 (CH_3 , 12-C), 123.80 (CH , 7-C), 125.01 (CH , 4-C), 130.09 (C_q , 3-C), 137.62 (C_q , 6-C), 164.92 (C_q , 2-C), 167.59 (C_q , 8-C), 174.27 (C_q , 11-C).

IR (neat): 583 (w), 662 (w), 693 (w), 722 (w), 758 (s), 866 (w), 905 (w), 1000 (w), 1059 (m), 1162 (s), 1199 (m), 1233 (s), 1252 (s), 1312 (w), 1351 (w), 1371 (w), 1437 (m), 1456 (w), 1520 (m), 1563 (m), 1680 (s), 1705 (s), 3348(br)

HRMS-ESI (m/z): Calculated for $[C_{17}H_{22}N_2O_7Na]^+$: 389.1319, found: 389.1319.

Melting point: 139.2°C (EtOAc)

2-aminoacetamido isophthalic acid dimethylester (4)



To a stirred solution of (**2**) (300 mg, 0.82 mmol) in 20 ml of CH₂Cl₂ was added 1 mL of trifluoroacetic acid. The resulting yellow solution was stirred for 12 h at room temperature. After that time the solvent was removed in vacuo and the product was obtained.

Yield: 299 mg (0.82 mmol, 100 %)

Empirical formula: C₁₂H₁₅N₂O₅ (colorless solid)

¹H-NMR (400 MHz, DMSO-d6, 298 K): δ = 3.78 (bs, 2H, 9-H), 3.82 (s, 6H, 1-H), 4.81 (bs, 2H, 10-H), 8.11 (s, 1H, 4-H), 8.38 (d, J = 1.5 Hz, 2H, 5-H), 10.94 (s, 1H, 7-H).

¹³C-NMR (75 MHz, DMSO-d6, 298 K): δ = 40.85 (CH₂, 9-C), 52.40 (2 CH₃, 1-C), 123.63 (CH, 4-C), 124.55 (2 CH, 5-C), 130.75 (2C_q, 3-C), 139.08 (C_q, 6-C), 164.90 (2C_q, 2-C), 165.49 (C_q, 8-C).

IR (neat): 613 (w), 757 (s), 793 (w), 874 (w), 904 (w), 935 (w), 1007 (m), 1108 (w), 1162 (w), 1209 (s), 1250 (s), 1315 (w), 1341 (m), 1440 (m), 1566 (w), 1617 (w), 1694 (m), 1715 (s), 2959 (w).

HRMS-ESI (m/z): Calculated for [C₁₂H₁₅N₂O₅H]⁺: 267.0975, found 267.0971

Melting point: 142.5°C (CH₂Cl₂)

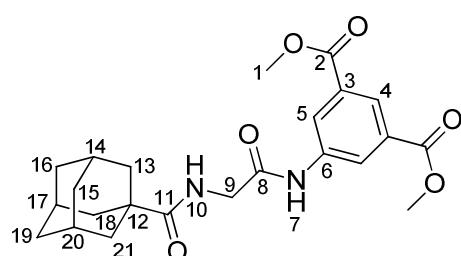
GP1 Coupling of diamondoid carboxyclic acids to (4)

To a stirred solution of the diamondoid structure in DMF were added EDCI and ethyl 2-cyano-2-(hydroxyimino) acetate. After stirring for 10 minutes (**4**) and NMM were added and the resulting solution was stirred for further 24 h at room temperature. The solvent was removed in vacuo and redissolved in CHCl₃. The organic layer was washed three times with water and saturated NaHCO₃. After drying over MgSO₄ and removal of the solvent the residue was treated with EtOAc. The resulting precipitate was filtered and washed several times with EtOAc. The crude compound was then purified via column chromatography (EtOAc / pentane 1:1).

GP2 Saponification

The protected diamondoid structure was dissolved in 2 mL of a mixture consisting of MeOH, THF and H₂O (1:1:2). After addition of NaOH pellets the resulting solution was stirred for 3 h at room temperature. The solution was neutralized subsequently using acidic ion exchange resin (Dowex HWCR 20), filtered and the solvent was removed in vacuo to obtain the desired product.

Adamantane-1-carboxamido acetamido-isophthalic acid dimethylester (7b)



According to GP1 adamantylcarboxylic acid (163 mg, 0.823 mmol), EDCI (174 mg, 0.905 mmol), 2-cyano-2-(hydroxyimino) acetate (155 mg, 0.905 mmol) were mixed in 10 mL DMF. After ten minutes (**4**) (138 mg, 0.905 mmol) and 0.1 mL of NMM were added.

Yield: 221 mg (0.522 mmol, 63 %)

Empirical formula: C₂₃H₂₈N₂O₆ (colorless solid)

¹H-NMR (400 MHz, DMSO-d6, 298 K): δ = 1.48-1.71 (m, 6H, 13,15,16-H), 1.78-1.91 (m, 6H, 18,19,21-H), 2.10-2.14 (m, 3H, 14,17,20-H), 3.93 (s, 6H, 1-H), 4.29 (d, J= 4.62 Hz, 2H, 9-H), 6.84 (t, J = 4.62 Hz, 1H, 10-H), 8.43 (t, J = 1.53 Hz, 1H, 4-H), 8.50 (d, J = 1.53 Hz, 2H, 5-H), 9.89 (s, 1H, 7-H).

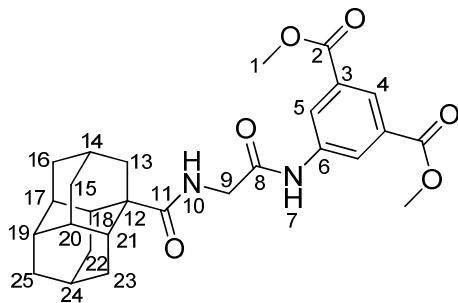
¹³C-NMR (101 MHz, DMSO-d6, 298 K): δ = 28.02 (CH, 14,17,20-C), 36.41 (CH₂, 13,18,20-C), 39.24 (CH₂, 15,16,19-C), 40.74 (CH₂, 9-C), 44.47 (C_q, 12-C), 52.46 (CH₃, 1-C), 124.71 (CH, 5-C), 126.34 (CH, 4-C), 131.32 (C_q, 3-C), 138.66 (C_q, 6-C), 165.93 (C_q, 2-C), 167.66 (C_q, 8-C), 179.34 (C_q, 11-C).

IR (neat): 613 (w), 640 (w), 755 (s), 793 (w), 871 (w), 902 (m), 1107 (m), 1196 (m), 1242 (s), 1340 (m), 1370 (m), 1431 (m), 1511 (s), 1586 (s), 1633 (s), 1702 (m), 1727 (s), 2856 (w), 2899 (br), 3108 (br), 3249 (w), 3279 (w), 3419 (m).

HRMS-ESI (m/z): Calculated. for [C₂₃H₂₈N₂O₆Na]⁺: 451.1843, found : 451.1840.

Melting point: 234.1°C (EtOAc)

Diamantane-1-carboxamido acetamido-isophthalic acid dimethylester (8b)



According to GP1 1-diadamantylcarboxylic acid (50 mg, 0.23 mmol), EDCI (0.35 mmol), 2-cyano-2-(hydroxyimino) acetate (0.35 mmol) were mixed in 10 mL DMF. After ten minutes (**4**) (93 mg, 0.35 mmol) and 0.1 mL of NMM were added.

Yield: 51 mg (0.11 mmol, 48 %)

Empirical formula: C₂₇H₃₂N₂O₆ (colorless solid)

¹H-NMR (400 MHz, DMSO-d6, 298 K): δ = 1.44-1.52 (m, 2H, 22, 23-H), 1.64-1.78 (m, 10H, 13,15,16,19,24,25-H), 1.86 (bs, 2H, 18,21-H), 1.90 (bs, 1H, 14-H), 1.95 (br s, 2H, 17-20-H), 2.19 (bs, 2H, 22,23-H), 3.93 (d, J = 5.8 Hz, 2H, 9-H), 3.95 (s, 6H, 1-H), 7.84 (t, J = 5.7 Hz, 1H, 10-H), 8.20 (t, J = 1.5 Hz, 1H, 4-H), 8.52 (d, J = 1.5 Hz, 2H, 5-H), 10.50 (s, 1H, 7-H).

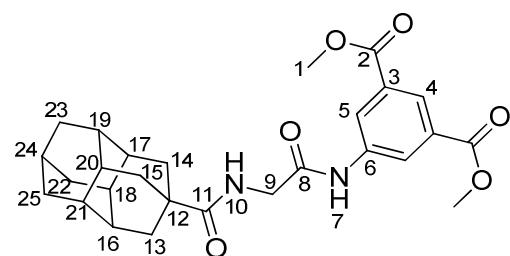
¹³C-NMR (101 MHz, DMSO-d6, 298 K): δ = 24.58 (CH, 24-C), 26.05 (CH, 14-C), 34.29 (CH, 15,16-C), 36.16 (CH, 19-C) 36.37 (C_q, 18,21-C), 37.11 (2 CH, 17,20-C), 37.49 (CH₂, 25-C), 42.11 (CH₂, 9-C), 42.62, (CH₂, 22,23-C), 45.73 (C_q, 12-C), 52.50 (2 CH₃, 1-C), 123.22 (2 CH, 5-C), 123.79 (CH, 4-C), 130.65 (2 C_q, 3-C), 139.95 (C_q, 6-C), 165,23 (C_q, 2-C), 168.77 (C_q, 8-C), 176.73 (C_q, 11-C).

IR (neat): 617 (w), 716 (w), 752 (s), 799 (w), 827 (w), 882 (w), 922 (w), 962 (w), 1002 (m), 1122 (m), 1197 (m), 1233 (m), 1315 (w), 1340 (m), 1369 (w), 1438 (m), 1508 (w), 1571 (w), 1632 (m), 1725 (s), 2874 (br), 2910 (br).

HRMS-ESI (m/z): Calculated. for [C₂₇H₃₂N₂O₆Na]⁺: 503.2153, found 503.2149

Melting point: 137.1°C (EtOAc)

Diamantane-4-carboxamido acetamido-isophthalic acid dimethylester (9b)



According to GP1 4-diadamantylcarboxylic acid (50 mg, 0.23 mmol), EDCI (0.35 mmol), 2-cyano-2-(hydroxyimino) acetate (0.35 mmol) were mixed in 10 mL DMF. After ten minutes (**4**) (93 mg, 0.35 mmol) and 0.1 mL of NMM were added.

Yield: 53 mg (0.12 mmol, 52 %)

Empirical formula: C₂₇H₃₂N₂O₆ (white solid)

¹H-NMR (400 MHz, DMSO-d6, 298 K): δ = 1.77-1.88 (m, 24H, 13-25H), 3.92 (d, *J* = 5.6 Hz, 2H, 9-H), 7.83 (t, *J* = 5.6 Hz, 1H, 10-H), 8.23 (s, 1H, 4-H), 8.50 (s, 2H, 5-H), 10.43 (s, 1H, 7-H).

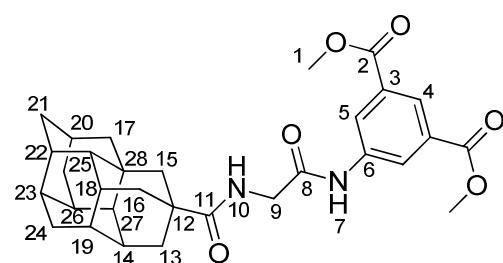
¹³C-NMR (101 MHz, DMSO-d6, 298 K): δ = 24.58 (CH, 24-C), 35.99 (CH, 18,19,21), 36.87 (CH, 22,23,25-C), 37.13 (CH, 16,17,20-C), 42.72 (C_q, 12-C), 45.74 (CH₂, 9-C), 52.50 (CH₃, 1-C), 123.33 (CH, 5-C), 123.93 (CH, 4-C), 130.66 (CH, 3-C), 140.03 (C_q, 6-C), 165.09 (C_q, 2-C), 168.64 (C_q, 8-C), 176.61 (C_q, 11-C).

IR (neat): 670 (w), 756 (s), 927 (w), 963 (w), 1001 (w), 1045 (w), 1103 (s), 1116 (m), 1197 (m), 1234 (s), 1315 (w), 1340 (w), 1368 (w), 1425 (m), 1509 (m), 1567 (m), 1636 (m), 1727 (s), 2909 (br).

HRMS-ESI (m/z): Calculated for [C₂₇H₃₂N₂O₆Na]⁺: 503.2153, found 503.2147

Melting point: 155.2°C (EtOAc)

Triamantane-9-carboxamido acetamido-isophthalic acid dimethylester (10b)



According to GP1 9-triadamantylcarboxylic acid (50 mg, 0.22 mmol), EDCI (0.33 mmol), 2-cyano-2-(hydroxyimino) acetate (0.33 mmol) were mixed in 10 mL DMF. After ten minutes (**4**) (88 mg, 0.33 mmol) and 0.1 mL of NMM were added.

Yield: 48 mg (0.09 mmol, 41%).

Empirical formula: C₃₁H₃₆N₂O₆ (white solid)

¹H-NMR (300 MHz, DMSO-d6, 298 K): δ = 1.03 (d, J = 2.5 Hz, 2H), 1.10 (s, 2H,), 1.16 (bs, 2H), 1.30-1.51 (m, 18H), 3.58 (d, J = 5.7 Hz, 2H, 9-H), 3.63 (s, 6H, 1-H), 7.48 (t, J = 5.7 Hz, 1H, 10-H), 7.89 (d, J = 1.4 Hz, 1H, 4-H), 8.21 (d, J = 1.4 Hz, 2H, 5-H), 10.17 (s, 1H, 7-H).

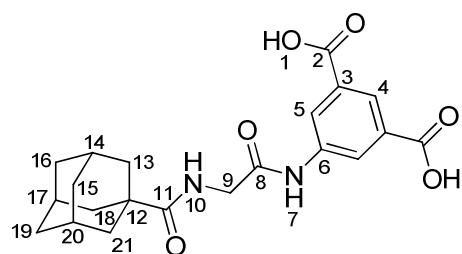
¹³C-NMR (75 MHz, DMSO-d6, 298 K): δ = 26.99 (CH, 20-C), 33.09 (CH₂, 24-C), 33.65 (CH₂, 21-C), 34.28 (CH, 28-C), 36.99 (2 CH, 18,19-C), 37.40, 37.43, 37.49, 37.55, 39.27, 39.81 (6 CH, 14,22,23,25,26,27-C), 42.72 (C_q, 12-C), 44.52 (CH₂, 17-C), 45.34 (CH₂, 9-C), 46.26 (2 CH₂, 13,16-C), 52.20 (2 CH₃, 1-C), 123.29 (CH, 5-C), 123.84 (CH, 4-C), 130.63 (CH, 3-C), 139.90 (C_q, 6-C), 165.21 (C_q, 2-C), 168.22 (C_q, 8-C), 177.16 (C_q, 11-C).

IR (neat): 620 (w), 670 (w), 706 (w), 757 (s), 790 (m), 868 (w), 899 (m), 957 (w), 999 (m), 1025 (w), 1106 (w), 1234 (s), 1339 (m), 1370 (w), 1430 (m), 1459 (w), 1514 (m), 1568 (m), 1629 (m), 1698 (w), 1724 (s), 2843 (w), 2871 (w), 2900 (m), 3413 (w).

HRMS-ESI (m/z): Calculated. for [C₃₁H₃₆N₂O₆Na]⁺: 555.2468 , found 555.2466

Melting point: 255.5°C decomp. (EtOAc)

Adamantane-1-carboxamido acetamido-isophthalic acid (7c)



According to GP 2 the protected substituted compound (100 mg, 0.23 mmol) was dissolved in a mixture of MeOH, THF and H₂O (1:1:2) together with sodium hydroxide (100 mg , 4.3 mmol). After neutralization the title compound was obtained.

Yield: 88 mg (0.22 mmol, 94%)

Empirical formula: C₂₁H₂₄N₂O₆ (colorless solid)

¹H-NMR (300 MHz, DMSO-d6, 298 K): δ = 1.51-1.72 (m, 6H, 13,15,16-H), 1.79-1.89 (m, 6H, 18,19,21-H), 2.11-2.16 (m, 3H, 14,17,20-H), 3.33 (d, J=5.78 Hz, 2H, 9-H), 7.73 (t, J=5.78, 1H, 10-H), 8.14 (t, J=1.51 Hz, 1H, 4-H), 8.42 (d, J= 1.51 Hz, 2H, 5-H), 10.36 (s, 1H, 7-H), 13.22 (br, 2H, 1-H).

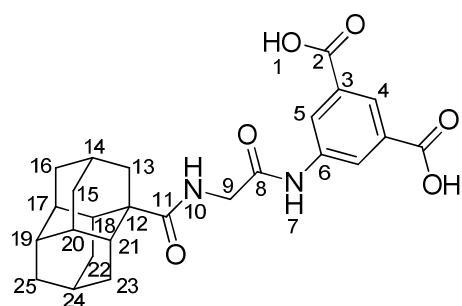
¹³C-NMR (75 MHz, DMSO-d6, 298 K): δ = 25.06 (CH , 14,17,20-C), 36.09 (CH₂, 13,18,20-C), 38.61 (CH₂, 15,16,19-C), 42.20 (CH₂, 9-C), 42.72 (Cq, 12-C), 109.49 (C_q), 123.29 (CH, 5-C), 124.37 (CH, 4-C), 131.68 (C_q, 3-C), 139.58 (C_q, 6-C), 166.42 (C_q, 2-C), 168.51 (C_q, 8-C), 177.46 (C_q, 11-C).

IR (neat): 686 (w), 752 (m), 1040 (w), 1108 (w), 1203 (m), 1275 (s), 1312 (w), 1366 (w), 1409 (m), 1431 (m), 1451 (m), 1513 /s), 1570 (m), 1606 (w), 1636 (s), 1712 (s), 2851 (br), 2907 (br).

HRMS-ESI (m/z): Calculated. for [C₂₁H₂₄N₂O₆Na]⁺ 423.1526, found 423.1527

Melting point: > 300°C (H₂O)

Diamantane-1-carboxamido acetamido-isophthalic acid (8c)



According to GP 2 the protected substituted compound (51 mg, 0.11 mmol) was dissolved in a mixture of MeOH, THF and H₂O (1:1:2) together with sodium hydroxide (100 mg , 4.3 mmol) of sodium hydroxide. After neutralization the title compound was obtained.

Yield: 46 mg (0.10 mmol, 92 %).

Empirical formula: C₂₅H₂₈N₂O₆ (colorless solid)

¹H-NMR (400 MHz, DMSO-d6, 298 K): δ = 1.45 (d, *J* = 12.4 Hz, 2H, 22,23-H), 1.64 – 1.69 (m, 10H, 13,15,16,19,24,25-H), 1.83 (bs, 2H, 18,19-H), 1.87 (bs, 1H, 14-H), 1.93 (bd, 2H, 17,20-H), 2.16 (s, 2H, 22,23-H), 3.89 (d, *J* = 5.8 Hz, 2H, 9-H), 7.80 (t, *J* = 5.8 Hz, 1H, 10-H), 8.17 (t, *J* = 1.5 Hz, 1H, 7-H), 8.43 (d, *J* = 1.5 Hz, 2H, 5-H), 10.38 (s, 1H, 7-H), 13.01 (bs, 2H, 1-H).

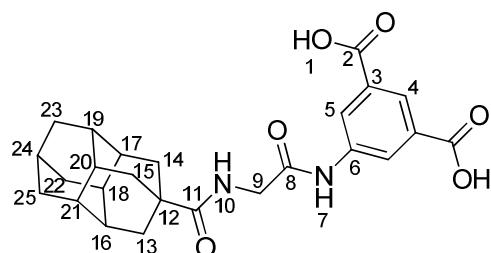
¹³C-NMR (75 MHz, DMSO-d6, 298 K): δ = 24.51 (CH, 24-C), 25.96 (CH, 14-C), 34.22 (2 CH₂, 15,16-C), 36.02 (CH, 19-C), 36.33 (2 CH₂, 22,23-C), 37.02 (CH₂, 25-C), 37.34 (2 CH, 17,20-C), 42.04 (CH₂, 9-C), 42.50 (2 CH₂, 22,23-C), 45.59 (C_q, 12-C), 122.38 (2 CH, 5-C), 122.85 (CH, 4-C), 132.93 (2 C_q, 3-C), 139.10 (C_q, 6-C), 166.96 (C_q, 2-C), 168.43 (C_q, 8-C), 177.15 (C_q, 11-C).

IR (neat): 669 (s), 703 (w), 757 (m), 807 (w), 899 (w), 951 (w), 1113 (w), 1134 (w), 1185 (s), 1243 (s), 1380 (m), 1439 (m), 1522 (m), 1567 (m), 1626 (w), 1682 (s), 1703 (s), 2892 (s), 3338 (m).

HRMS-ESI (m/z): Calculated for [C₂₅H₂₈N₂O₆Na]⁺: 475.1840, found 475.1839.

Melting point: > 300°C (H₂O)

Diamantane-4-carboxamido acetamido-isophthalic acid (9c)



According to GP 2 the protected substituted compound (54 mg, 0.12 mmol) were dissolved in a mixture of MeOH, THF and H₂O (1:1:2) together with sodium hydroxide (100 mg , 4.3 mmol). After neutralization the title compound was obtained.

Yield: 46 mg (0.10 mmol, 84 %).

Empirical formula: C₂₅H₂₈N₂O₆ (colorless solid).

¹H-NMR (300 MHz, DMSO, 298 K): δ = 1.77-1.88 (m, 24H, 13-25H), 3.92 (d, *J* = 5.6 Hz, 2H, 9-H, 7.83 (t, *J* = 5.6 Hz, 1H, 10-H), 8.23 (s, 1H, 4-H), 8.50 (s, 2H, 5-H), 10.43 (s, 1H, 7-H), 13.15 (bs, 2H, 1-H).

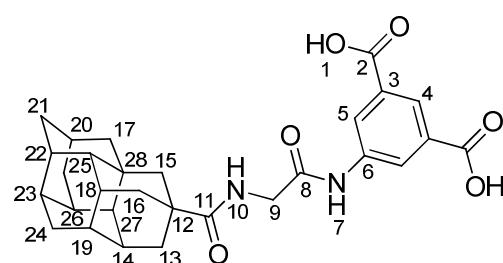
¹³C-NMR (75 MHz, DMSO, 298 K): δ = 24.92 (CH, 24-C), 35.89 (3 CH, 18,19,20-C), 36.76 (3 CH, 22,23,25-C), 37.04 (CH, 16,17,20-C), 37.93 (s), 39.40 (CH₂, 9-C), 42.67 (C_q, 12-C), 123.38 (CH, 4-C), 124.47 (CH, 4-C), 131.74 (CH, 3-C), 139.34 (C_q, 6-C), 166.48 C_q, 2-C), 168.51 (C_q, 8-C), 178.01 (C_q, 11-C).

IR (neat): 611 (w), 674 (s), 735 (m), 756 (m), 801 (w), 910 (w), 927 (w), 954 (w), 1031 (w), 1048 (w), 1117 (w), 1137 (w), 1191 (s), 1244 (m), 1282 (m), 1330 (w), 1376 (w), 1412 (m), 1524 (m), 1570 (w), 1600 (w), 1675 (s), 1703 (s), 2872 (s), 2900 (br), 3326 (m).

HRMS-ESI (m/z): Calculated for [C₂₅H₂₈N₂O₆Na]⁺: 475.1840, found 475.1833

Melting point: > 300°C (H₂O)

Triamantane-9-carboxamido acetamido-isophthalic acid (10c)



According to GP 2 the protected substituted compound (44 mg, 0.08 mmol) were dissolved in a mixture of MeOH, THF and H₂O (1:1:2) together with sodium hydroxide (100 mg , 4.3 mmol). After neutralization the title compound was obtained.

Yield: 36 mg (0.07 mmol, 89 %).

Empirical formula: (colorless solid)

¹H-NMR (300 MHz, DMSO, 298 K): 1.28 (d, *J* = 2.2 Hz, 2H), 1.35 (s, 2H),), 1.41 (s, 2H), 1.87 – 1.55 (m, 18H); 3.83 (d, *J* = 5.7 Hz, 2H, 9-H), 7.72 (t, *J* = 5.7 Hz, 1H, 10-H), 8.16 (s, 1H, 4-H), 8.43 (s, 2H, 5-H), 10.33 (s, 1H, 7-H), 13.21 (bs, 2H, 1-H).

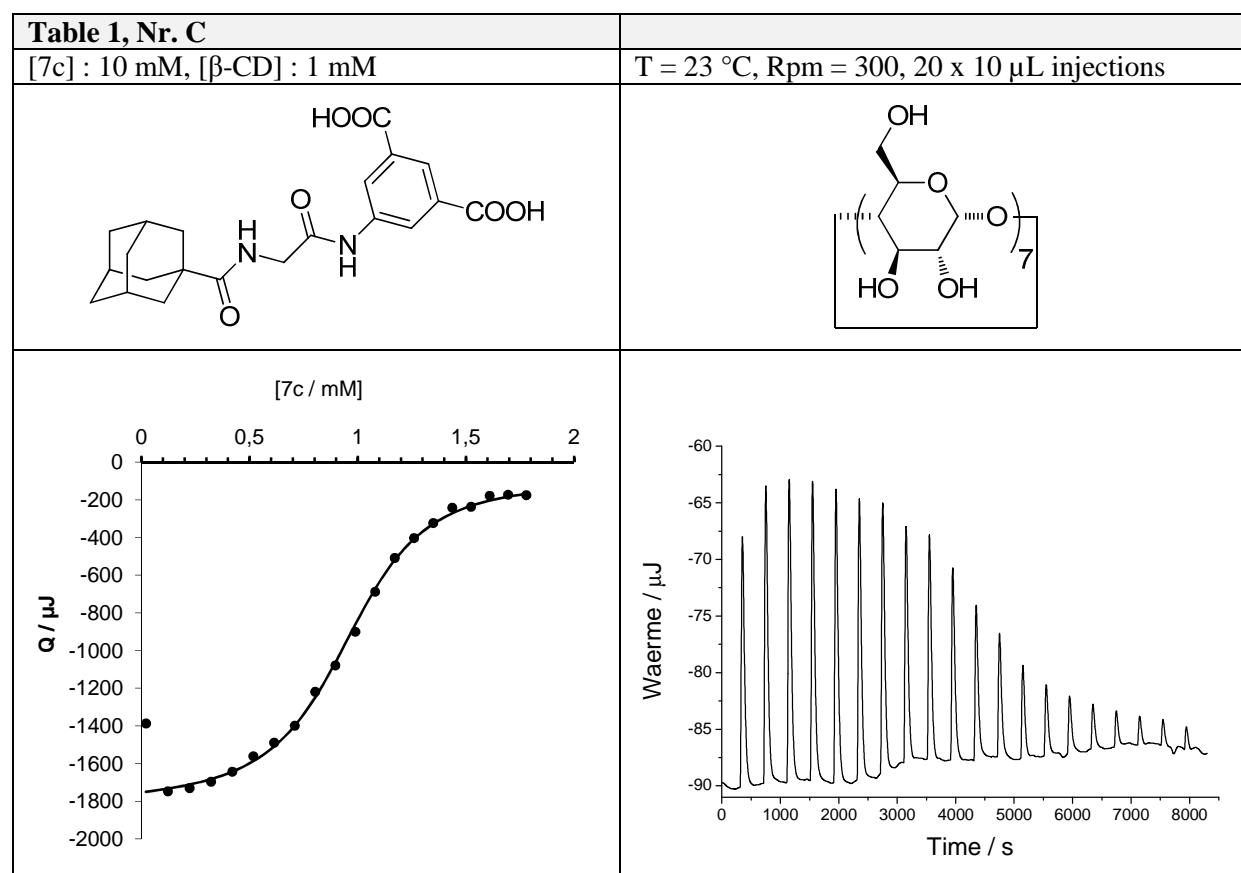
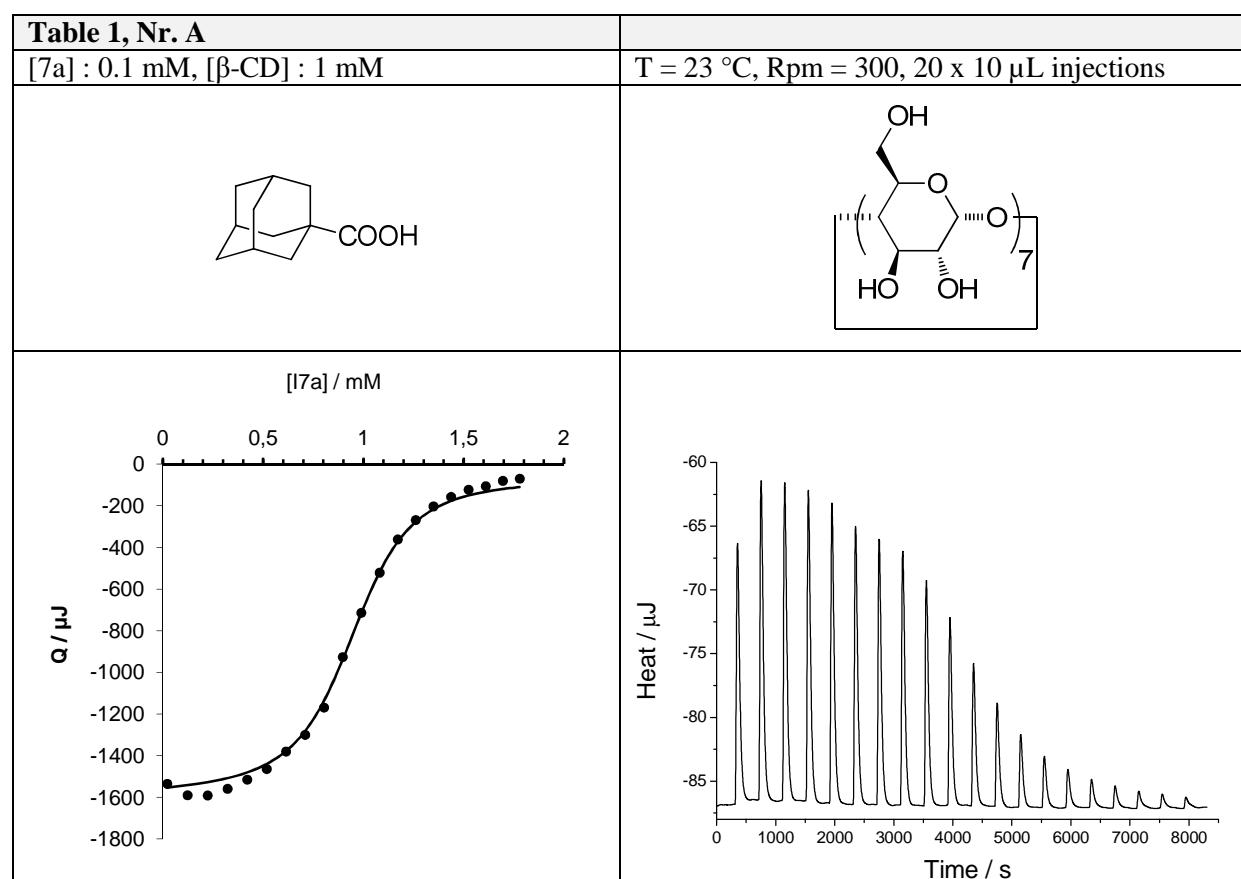
¹³C-NMR (75 MHz, DMSO, 298 K): δ = 27.03 (CH, 20-C), 33.13 (CH₂, 24-C), 33.69 (CH₂, 21-C), 34.37 (CH, 28-C), 37.03 (2 CH, 18,19-C), 37.44, 37.47, 37.50, 37.53, 39.24, 39.80 (6 CH, 14,22,23,25,27-C), 42.77 (C_q, 12-C), 44.55 (CH₂, 17-C), 45.38 (CH₂, 9-C), 46.32 (2CH₂, 13,16-C), 66.99 (CH₂, 15-C), 123.34 (CH, 5-C), 124.40 (CH, 4-C), 131.70 (CH, 3-C), 139.59 (C_q, 6-C), 166.41 (C_q, 2-C), 168.51 (C_q, 8-C), 177.18 (C_q, 11-C).

IR (neat): 585 (w), 691 (m), 760 (s), 908 (w), 953 (w), 1023 (w), 1199 (m), 1261 (s), 1279 (s), 1366 (w), 1410 (m), 1437 (s), 1508 (m), 1572 (m), 1601 (m), 1692 (s), 2846 (br), 2899 (s), 3116 (w).

HRMS-ESI (m/z): Calculated for [C₂₉H₃₂N₂O₆Na]⁺: 527.2153, found 527.2156.

Melting point: > 300°C (H₂O)

2. Isothermal titration calorimetry (ITC)



Electronic Supplementary Information: Nanodiamonds in Sugar Rings

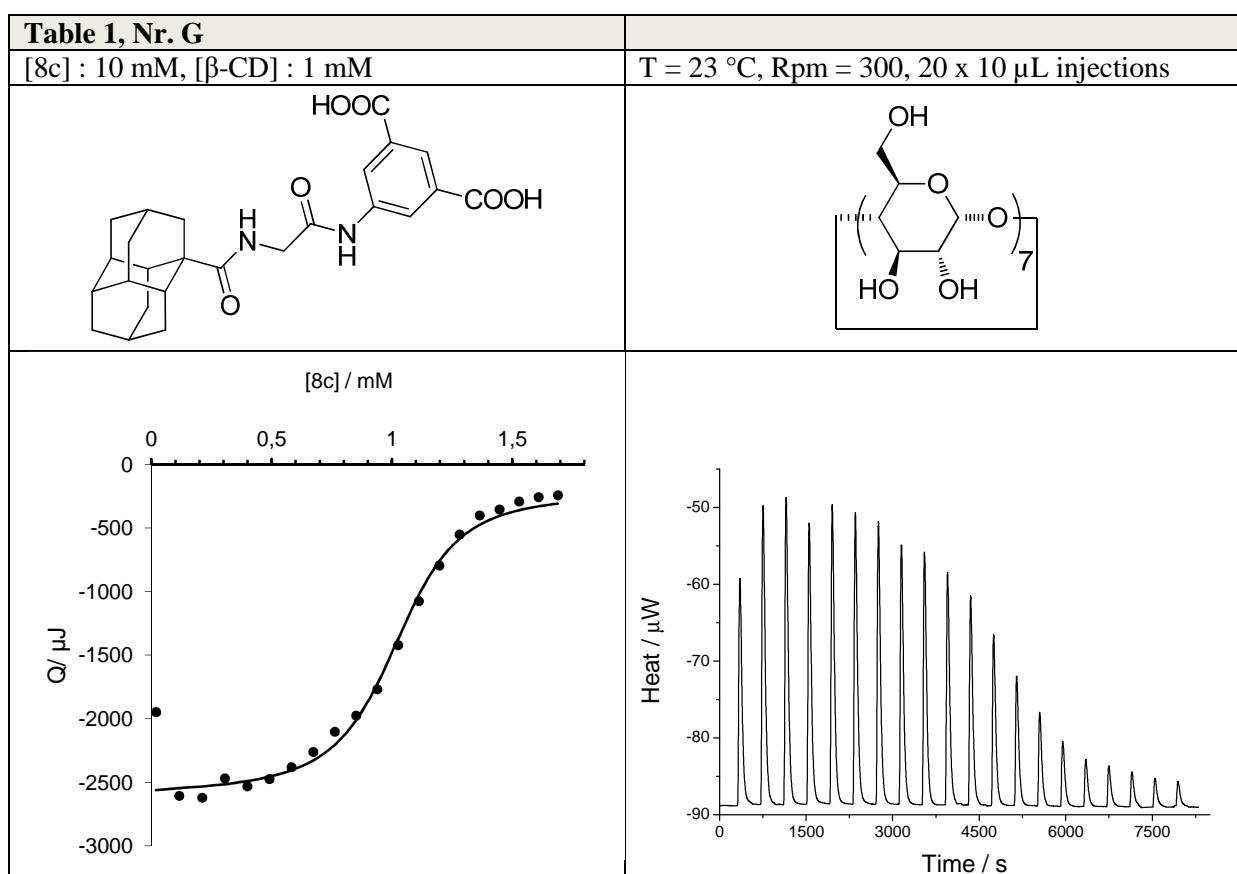
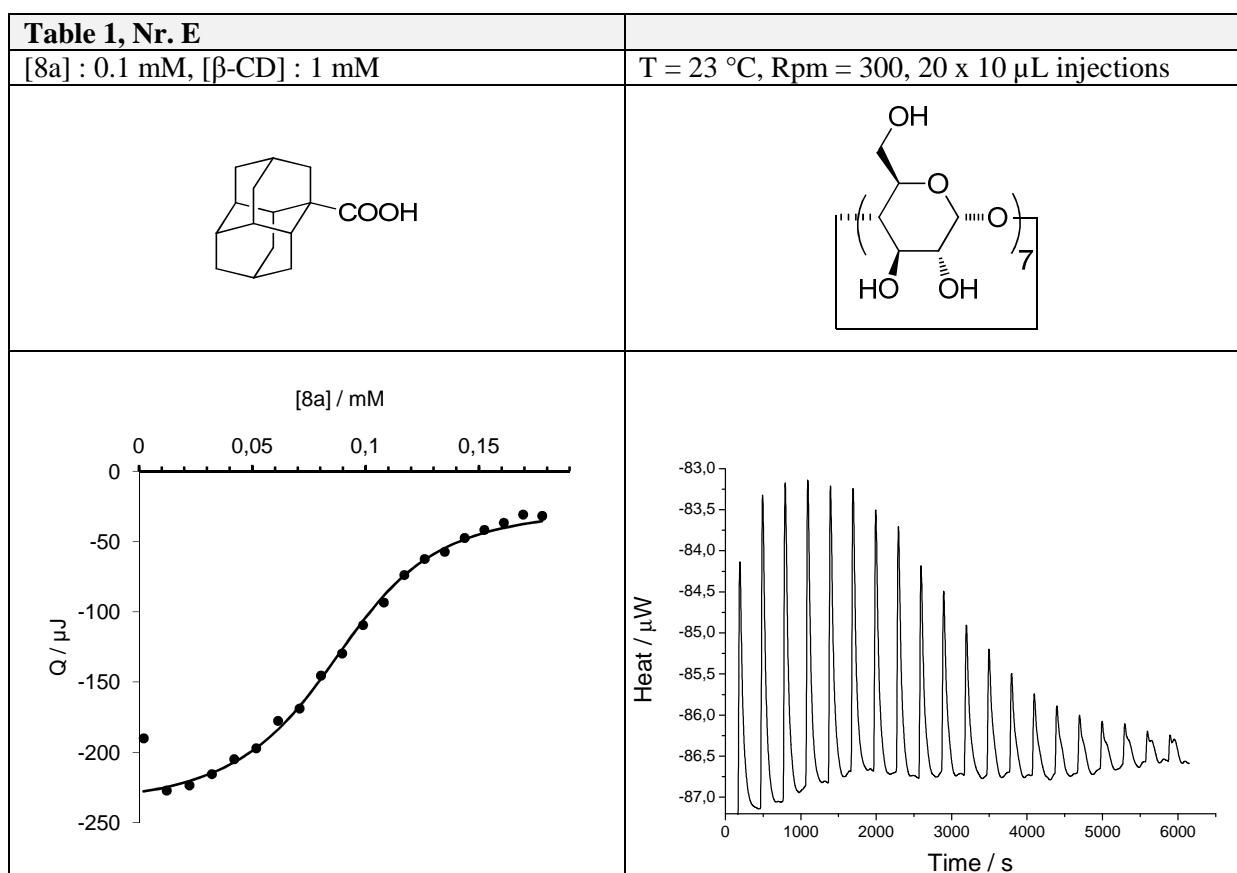


Table 1, Nr. H

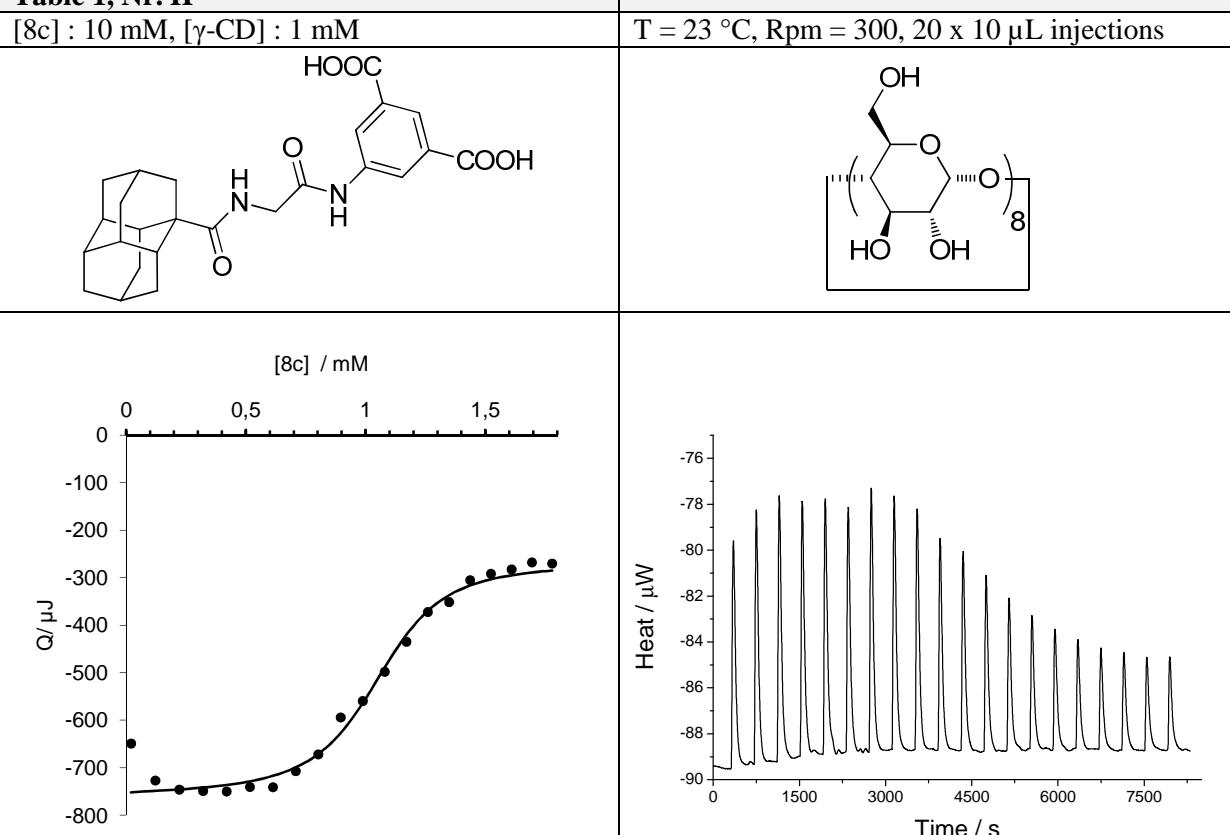
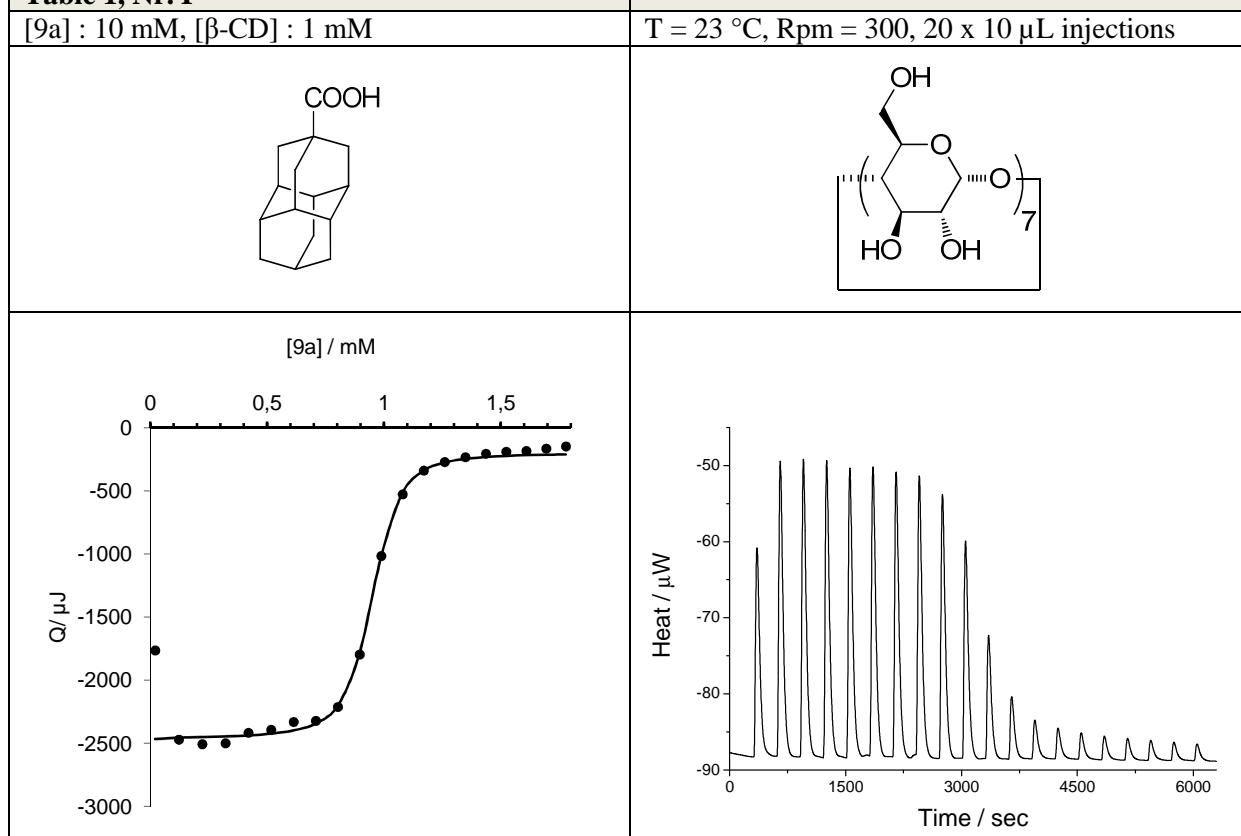
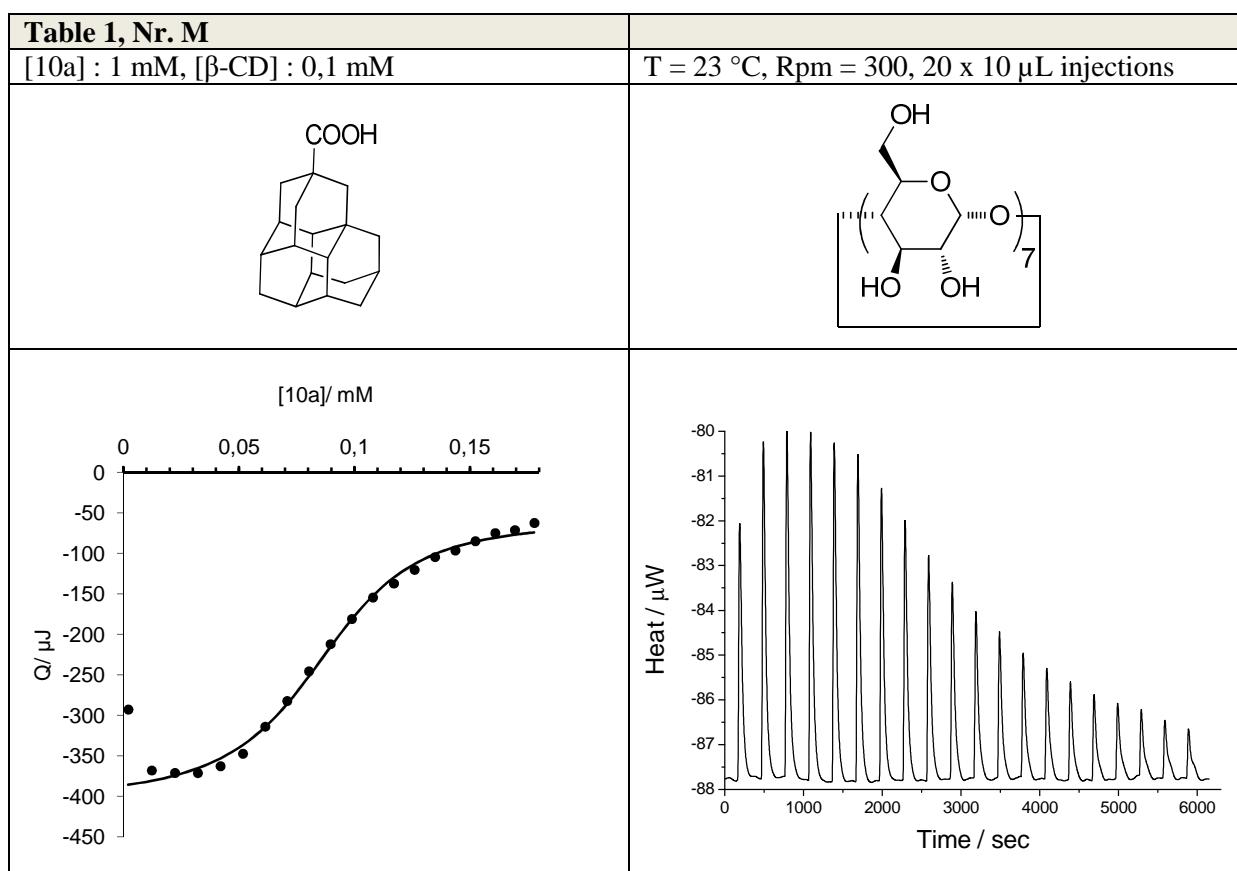
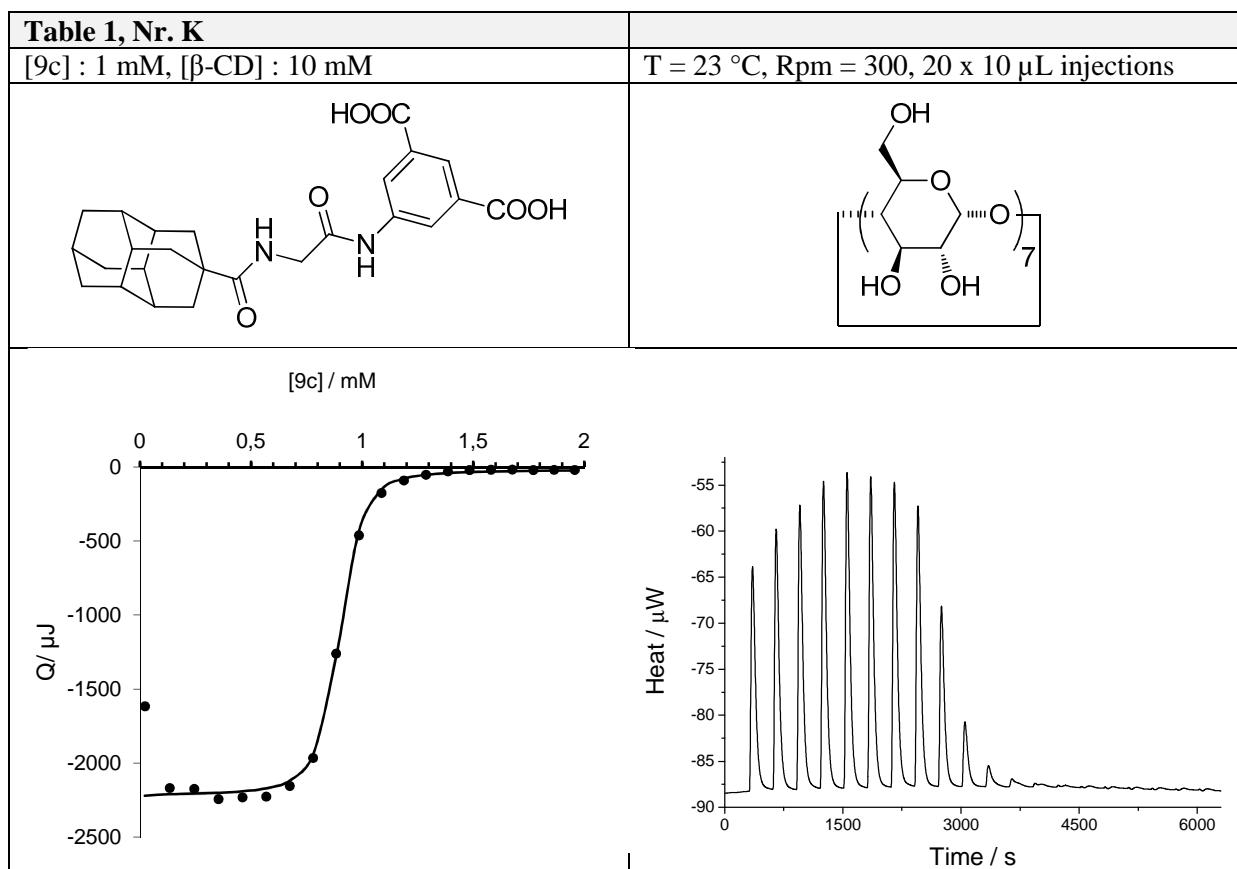
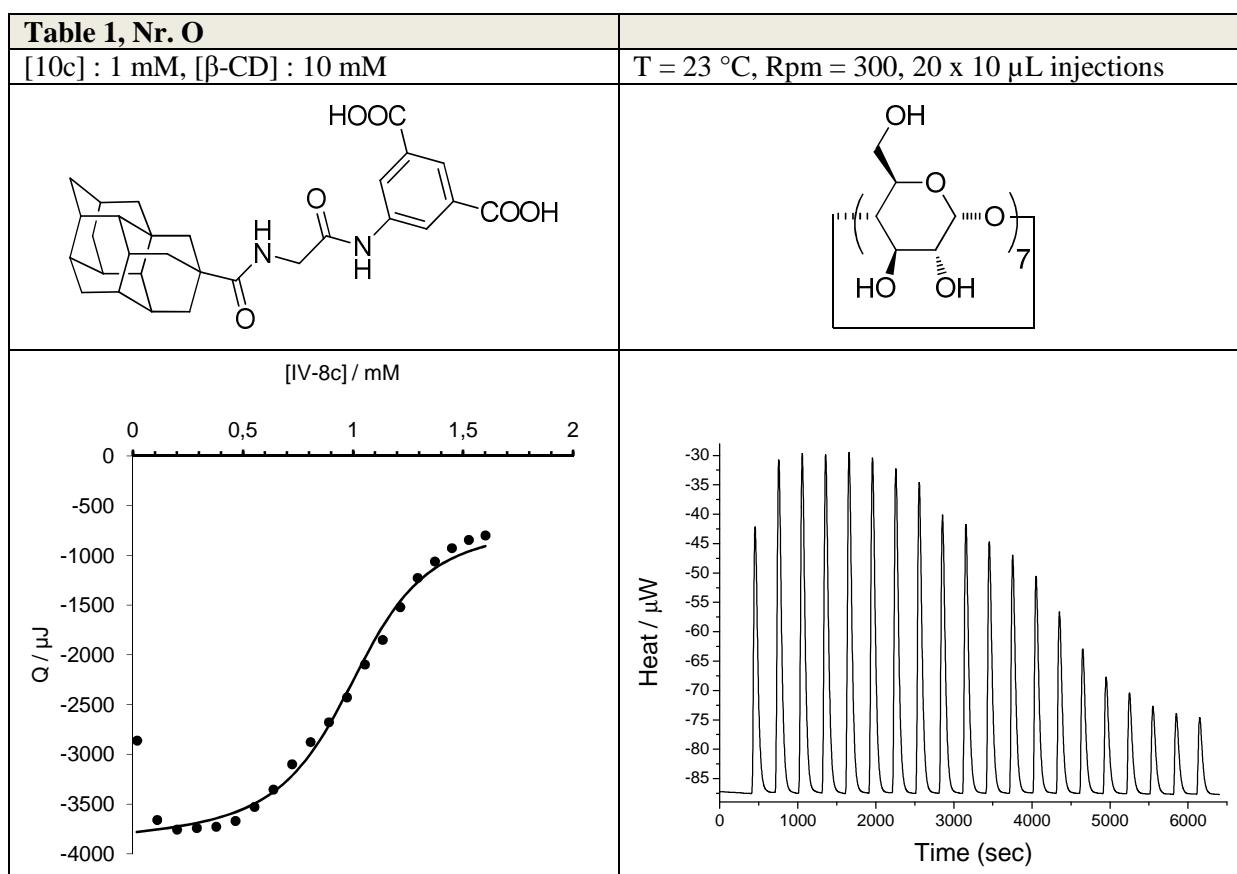
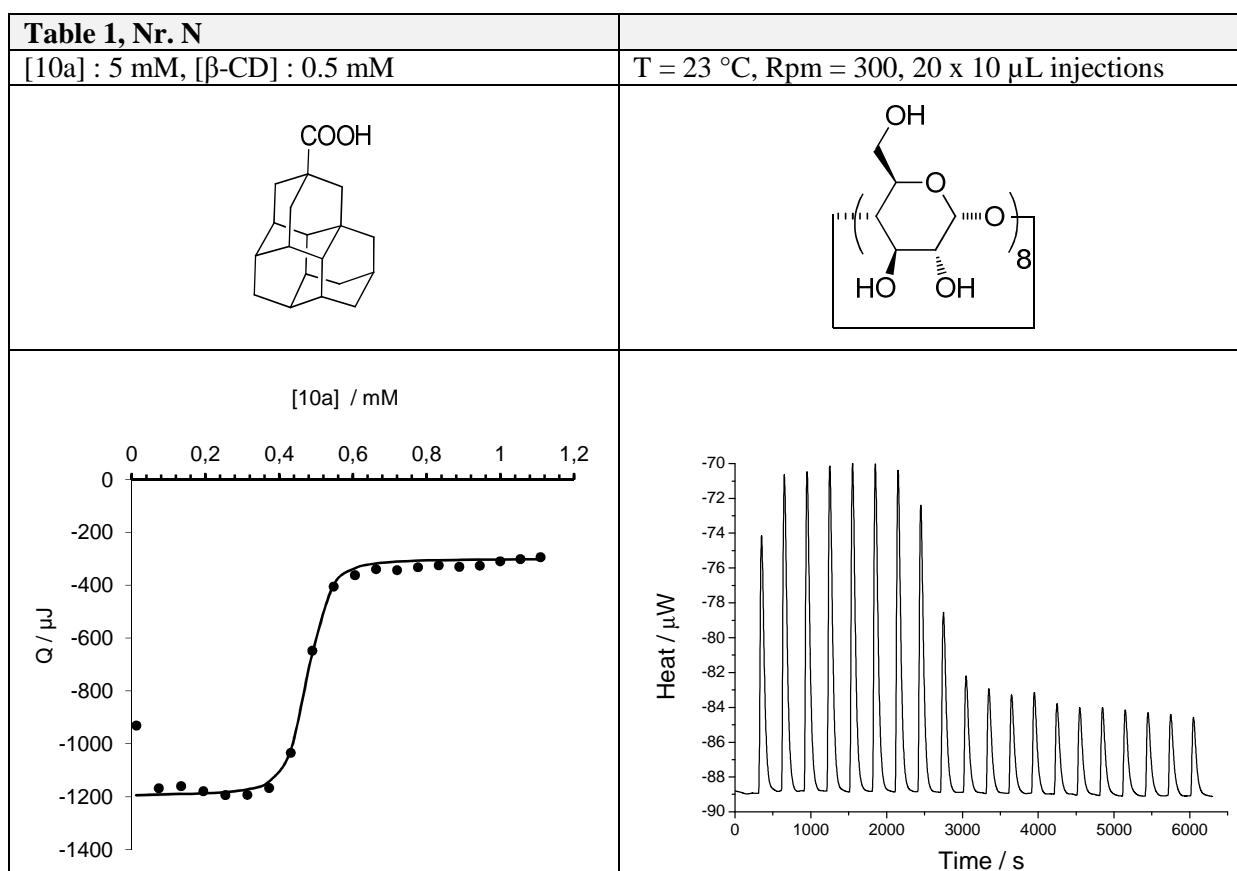


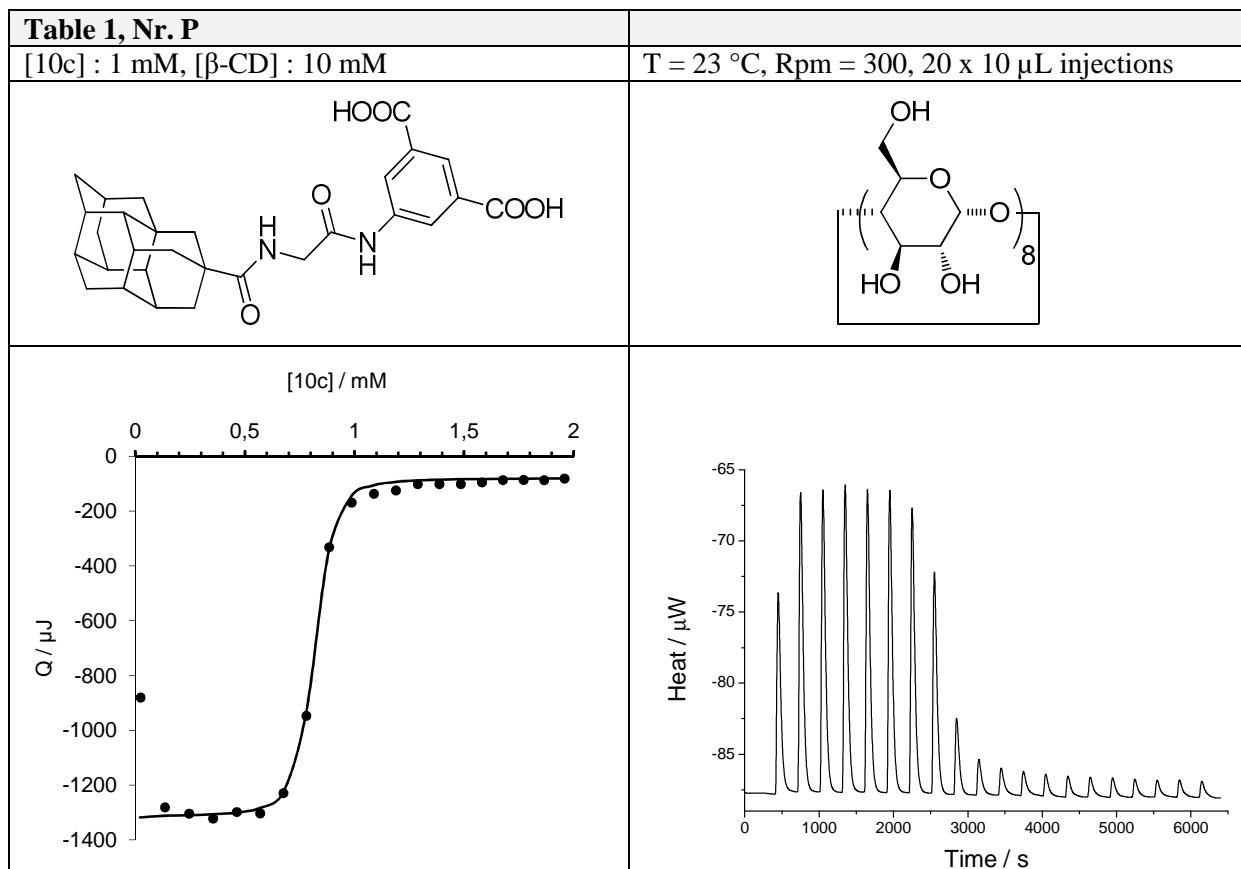
Table 1, Nr. I



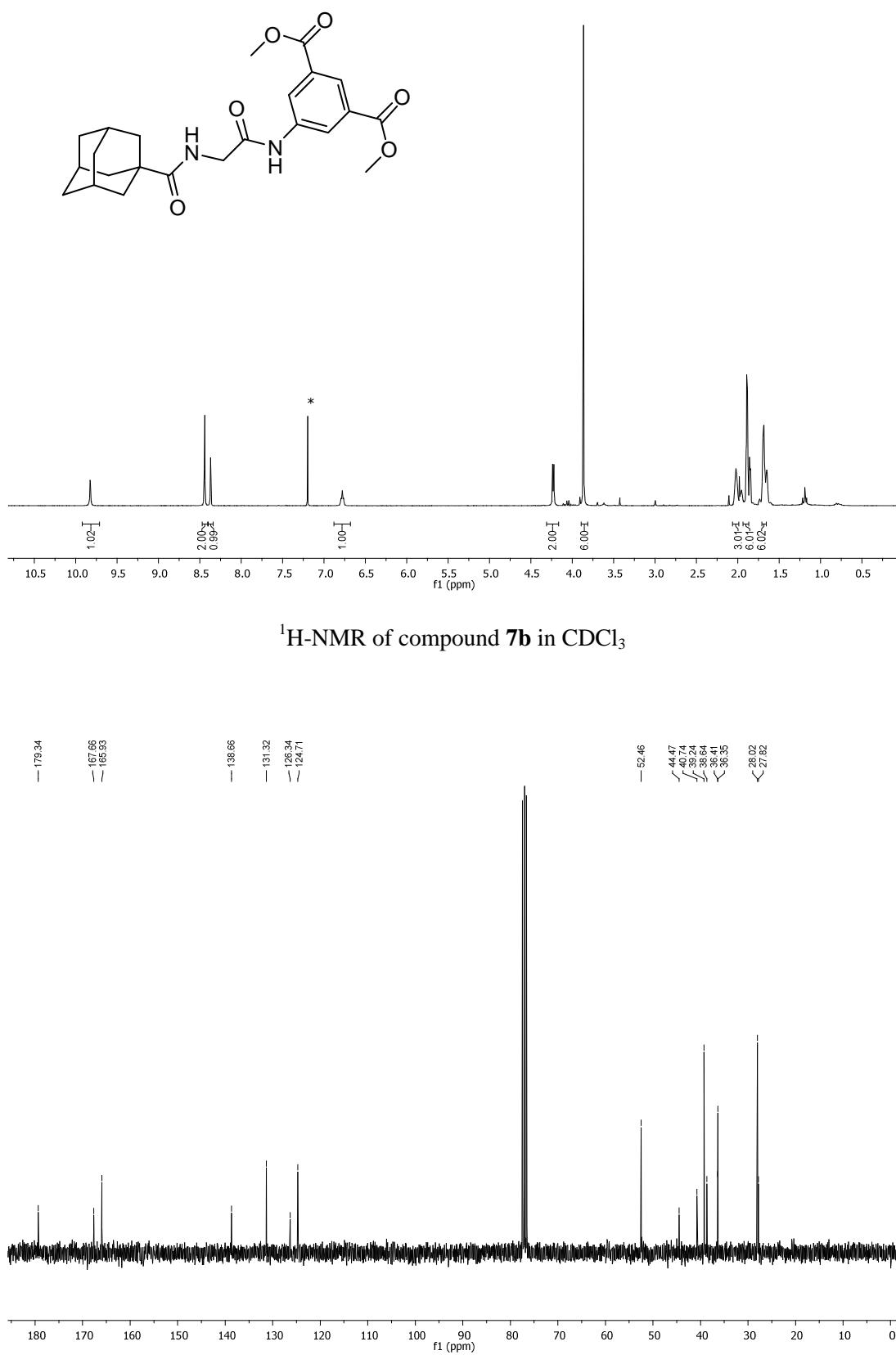


Electronic Supplementary Information: Nanodiamonds in Sugar Rings



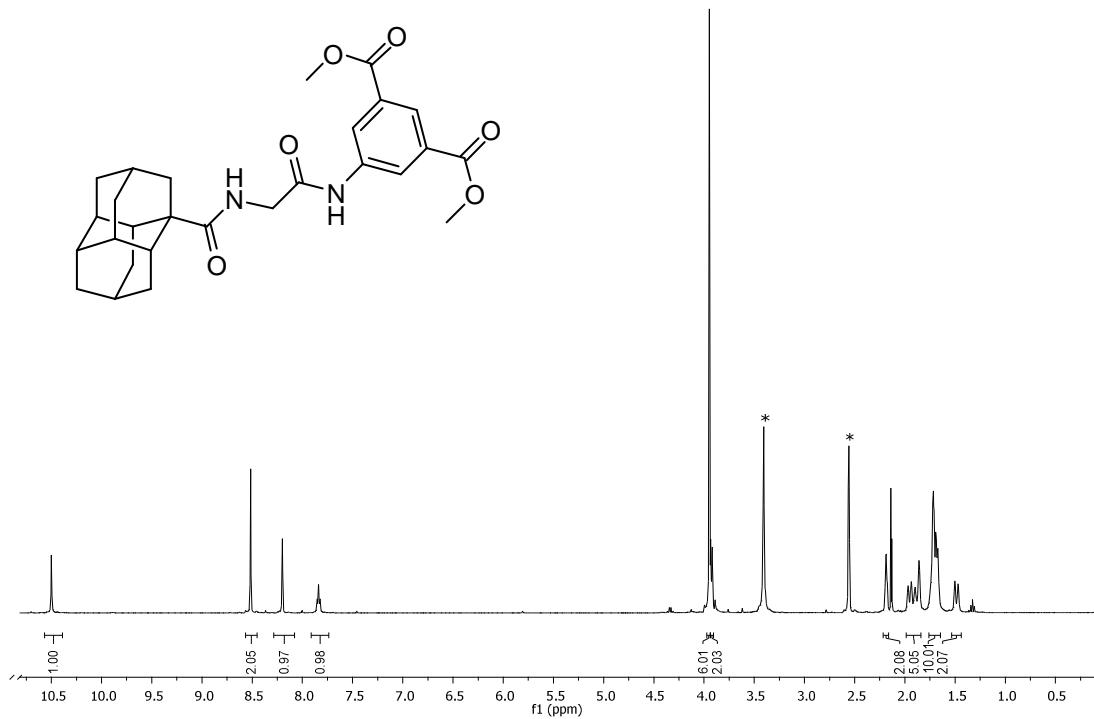
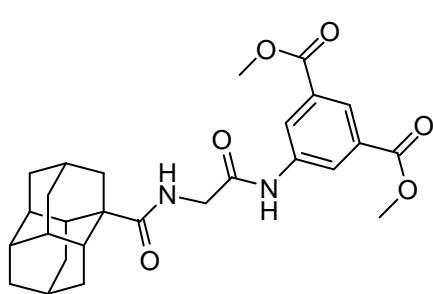


3. NMR Spectra

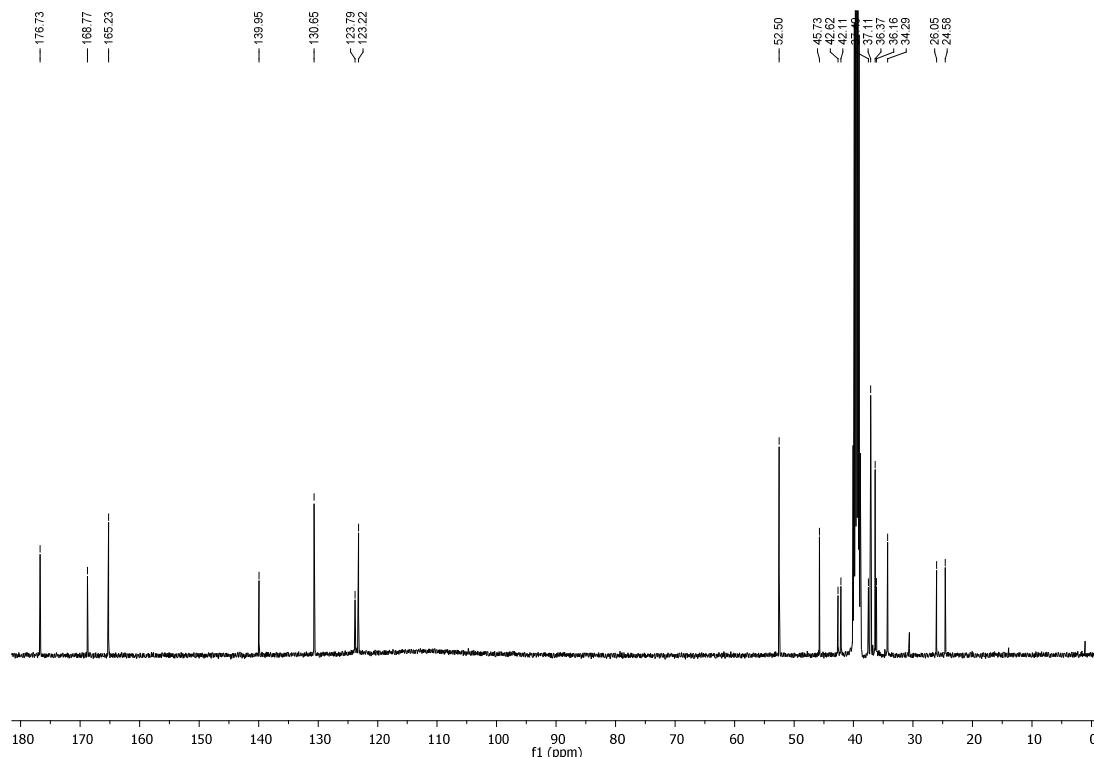


¹H-NMR of compound **7b** in CDCl₃

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

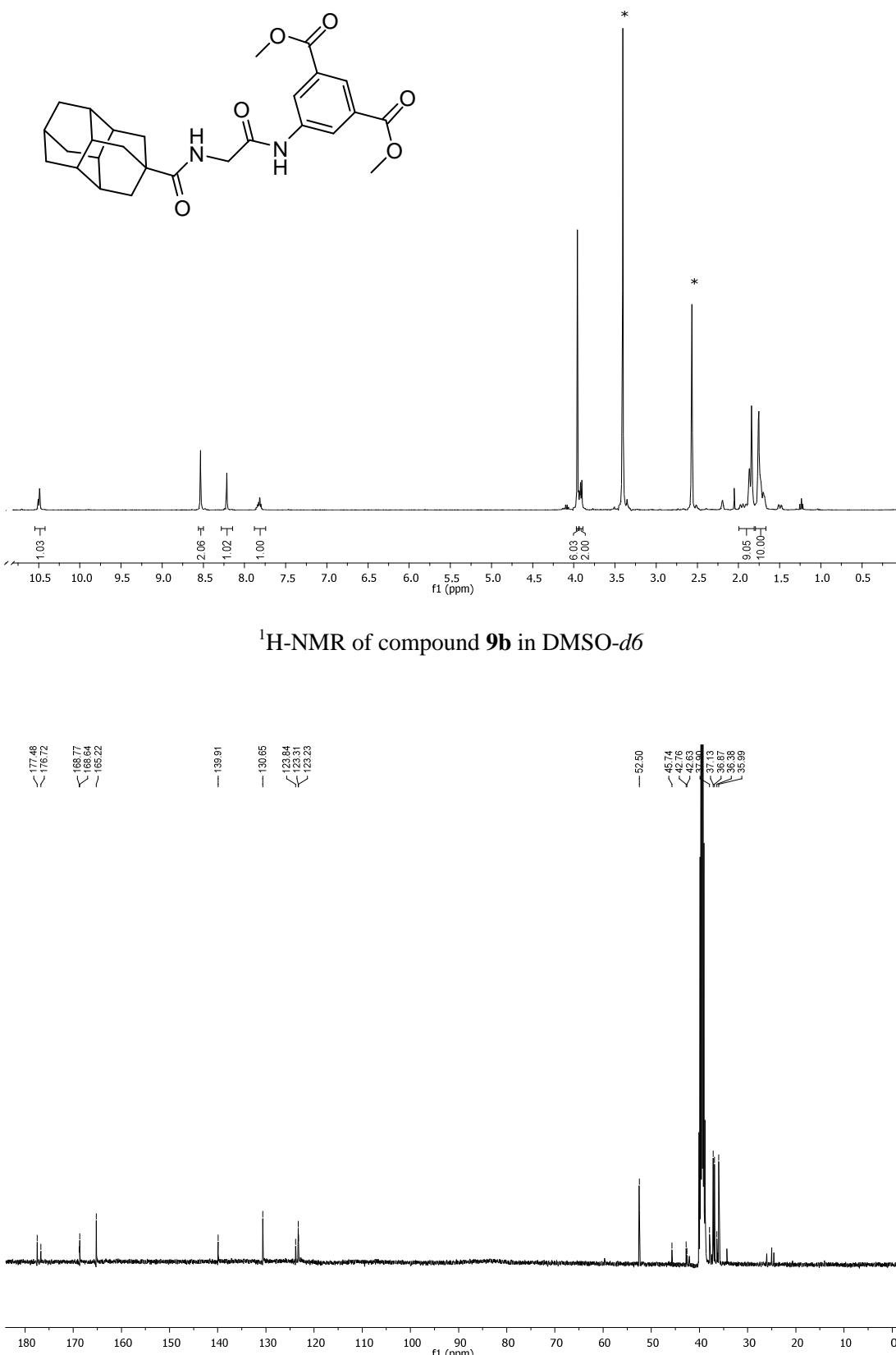


^1H -NMR of compound **8b** in $\text{DMSO}-d_6$

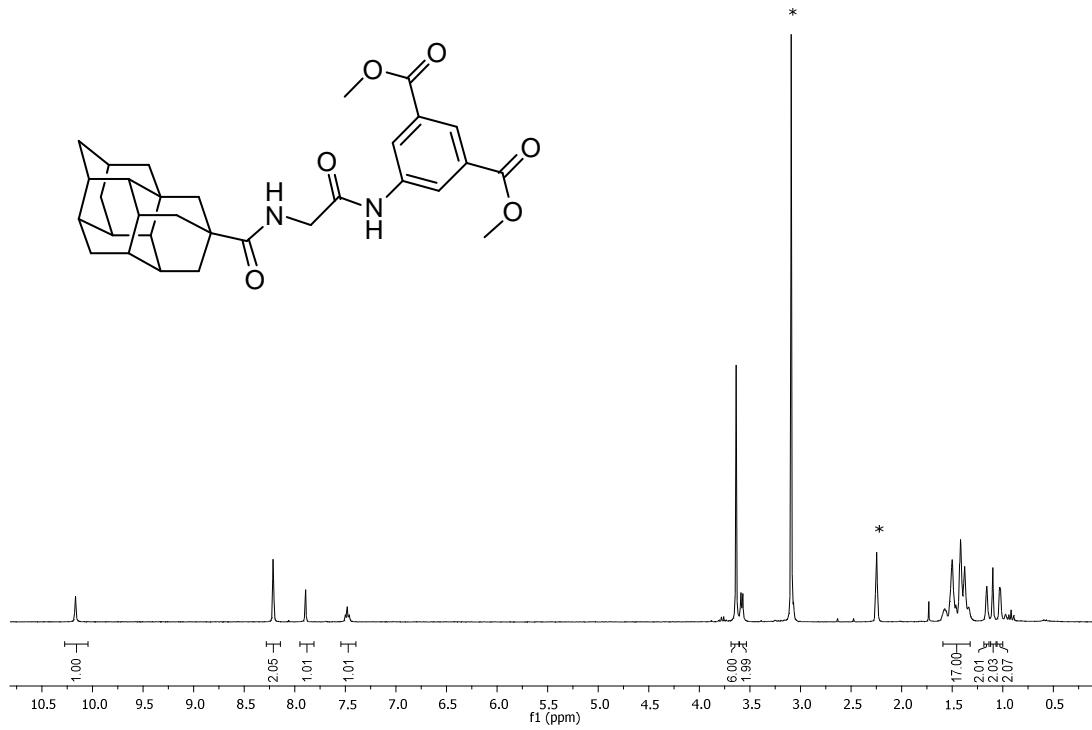
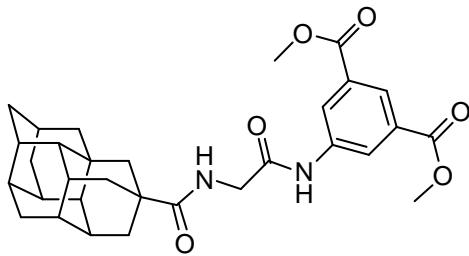


^{13}C -NMR of compound **8b** in $\text{DMSO}-d_6$

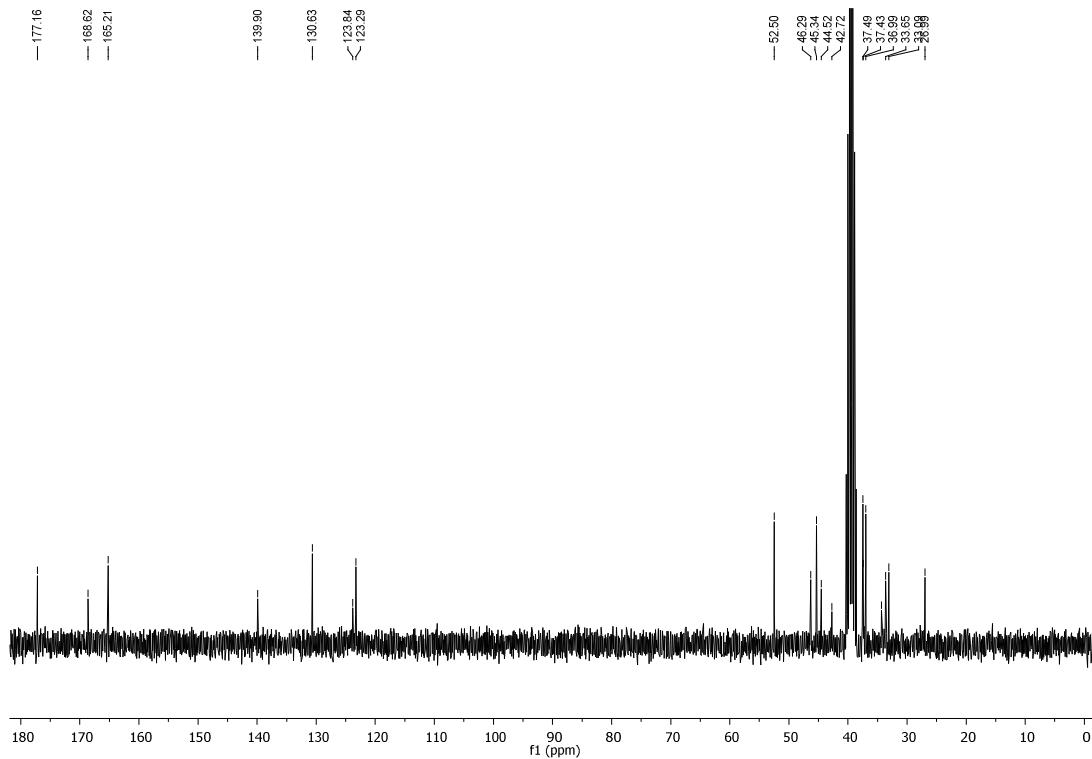
Electronic Supplementary Information: Nanodiamonds in Sugar Rings



¹H-NMR of compound **9b** in DMSO-*d*6

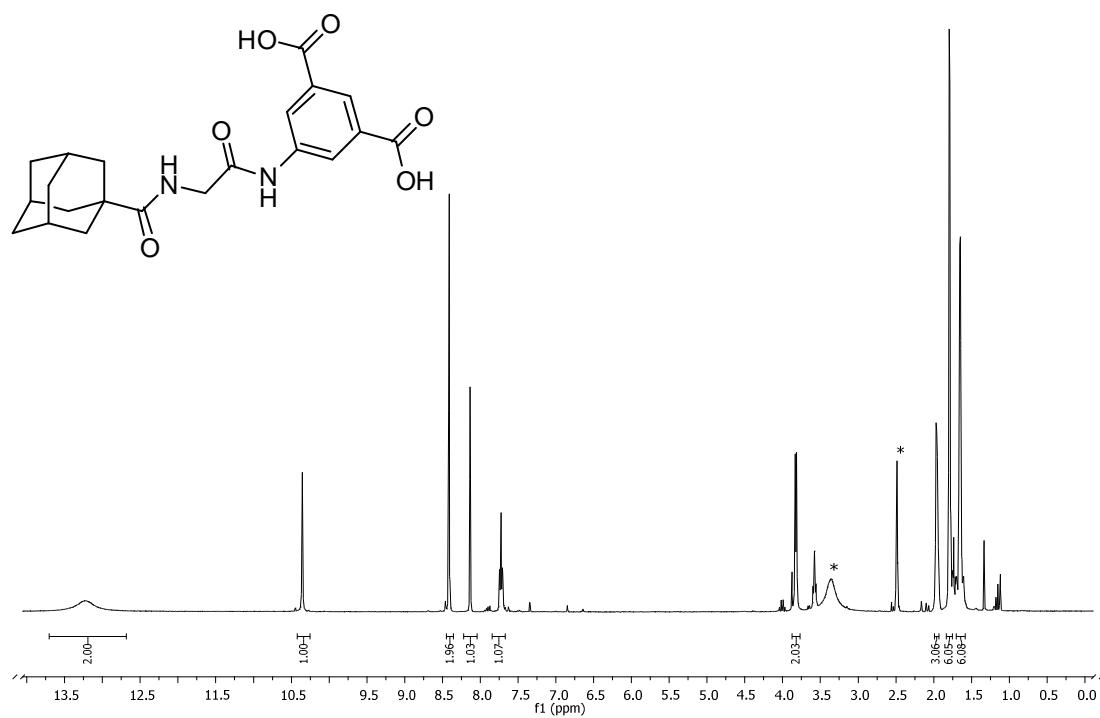


¹H-NMR of compound **10b** in DMSO-*d*6

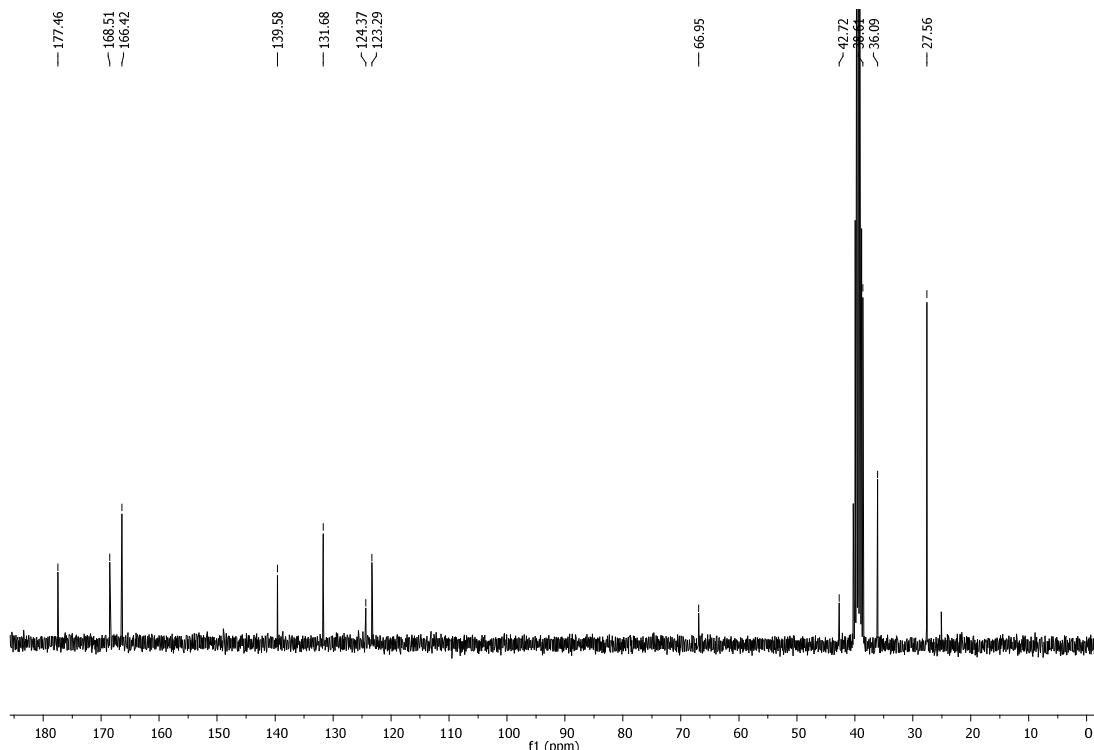


¹³C-NMR of compound **10b** in DMSO-*d*6

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

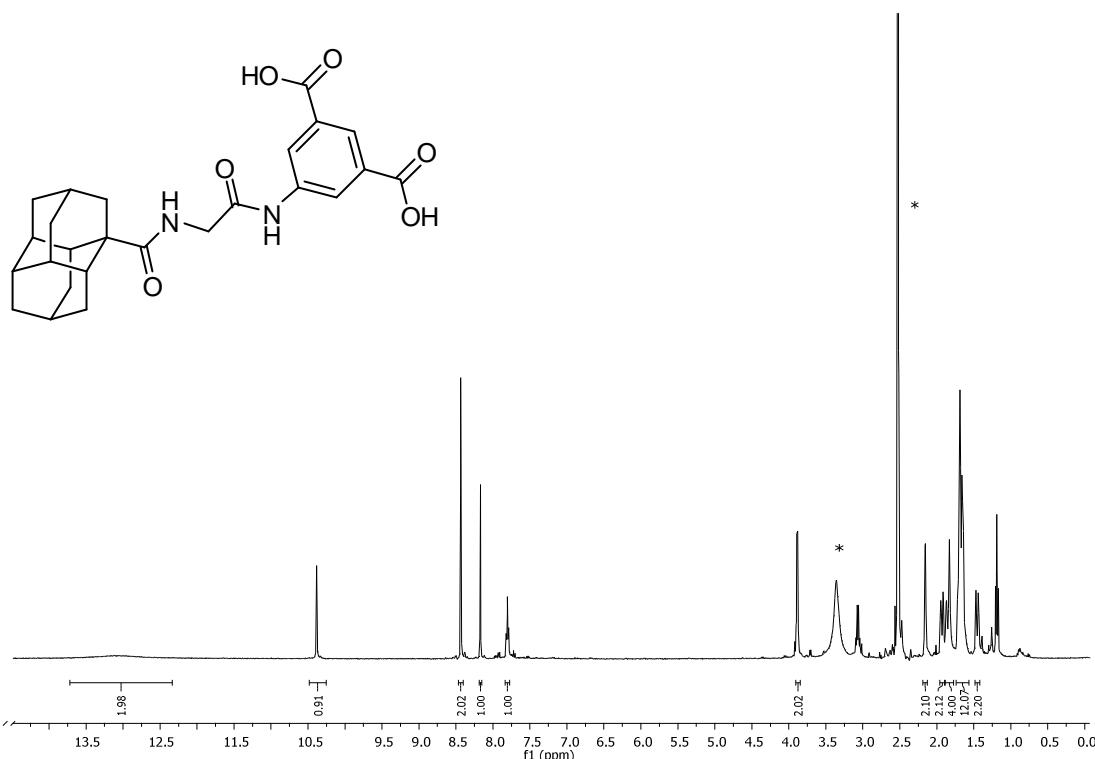


¹H-NMR of compound 7c in DMSO-*d*6

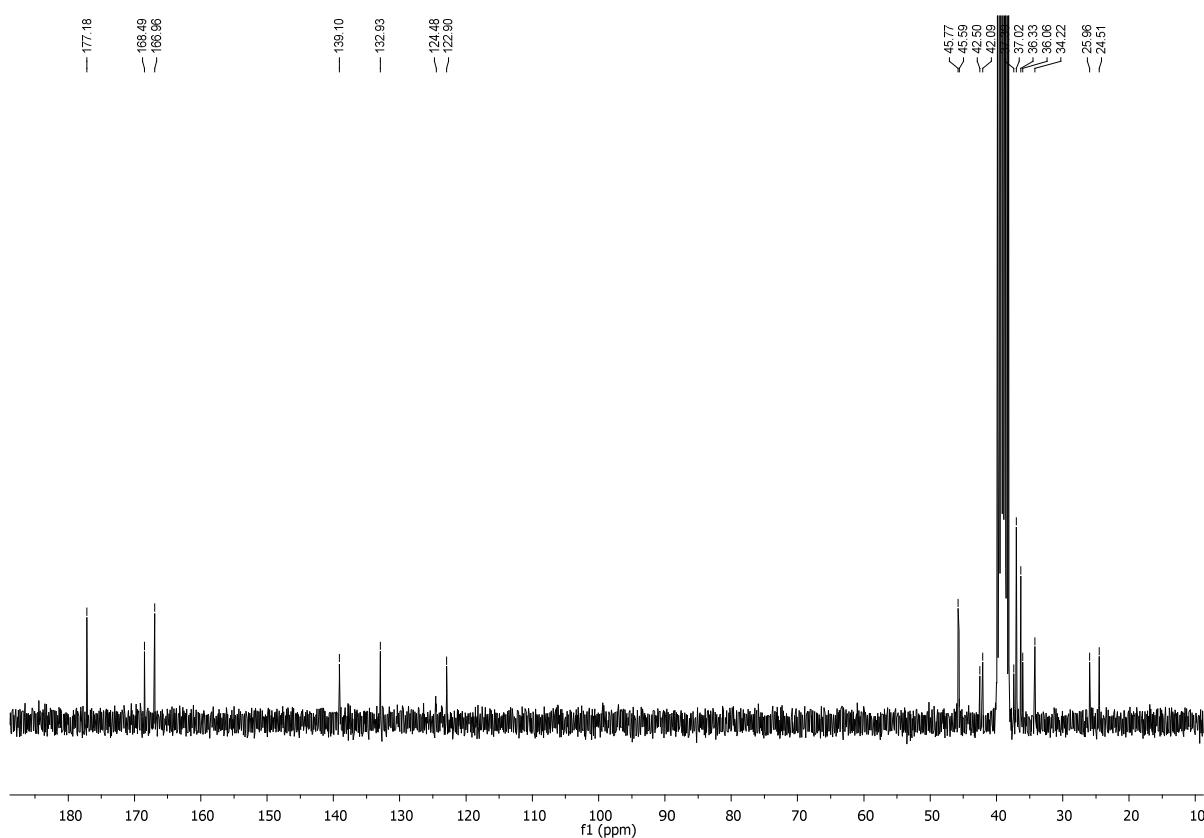


¹³C-NMR of compound 7c in DMSO-*d*6

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

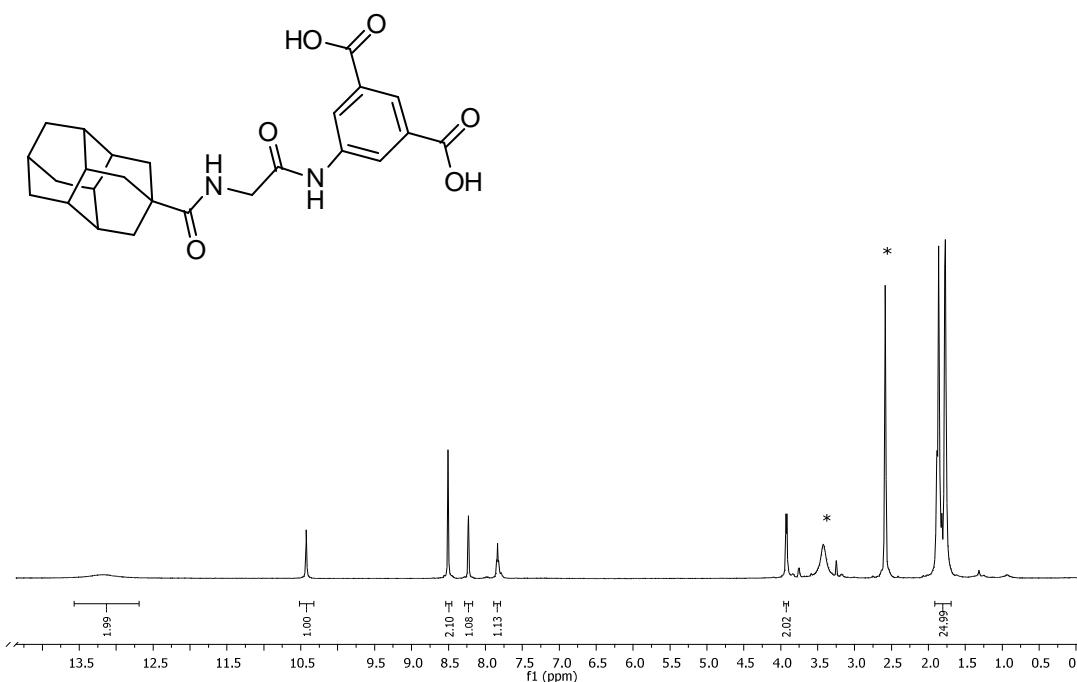


¹H-NMR of compound **8c** in DMSO-*d*6

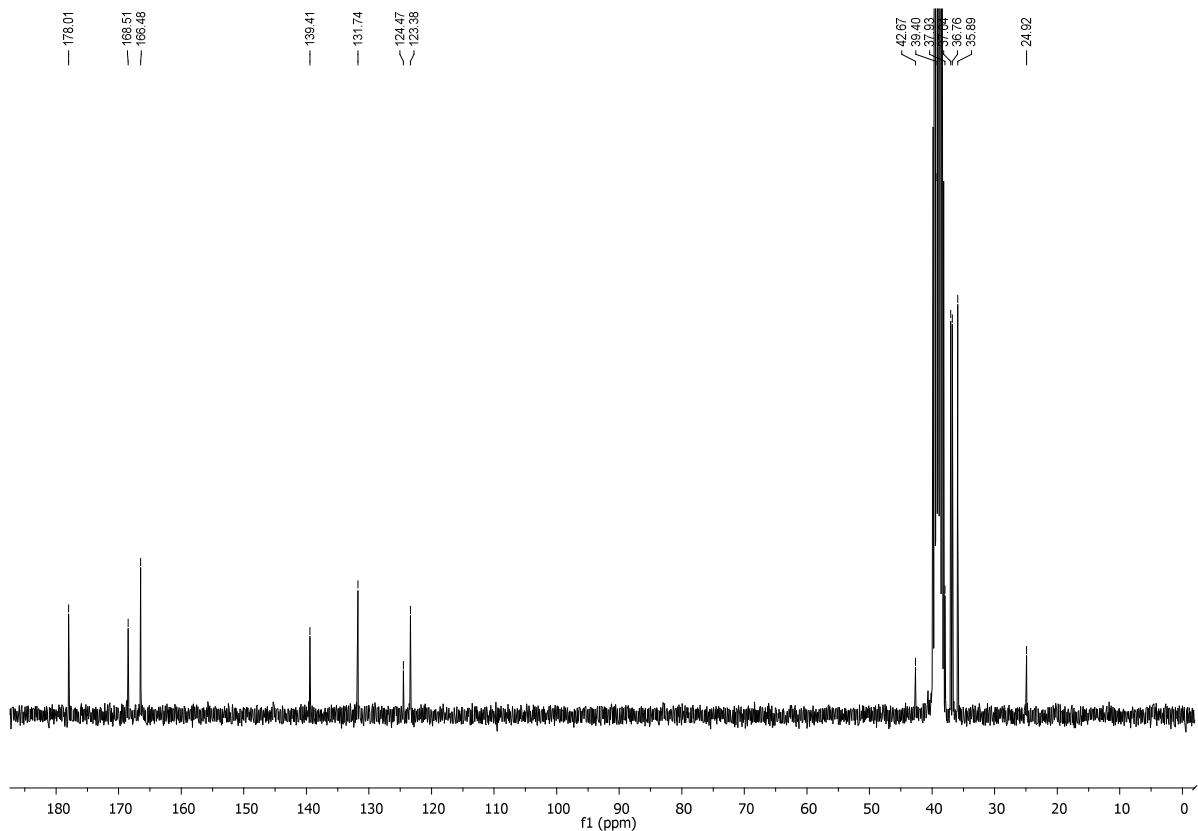


¹³C-NMR of compound **8c** in DMSO-*d*6

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

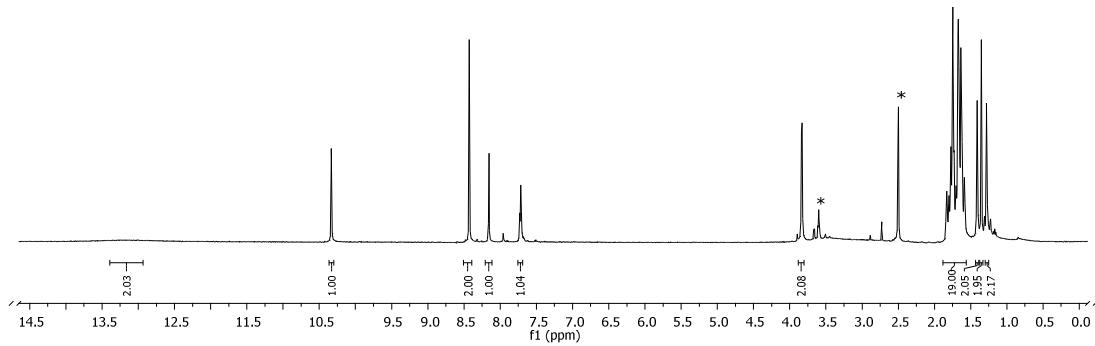
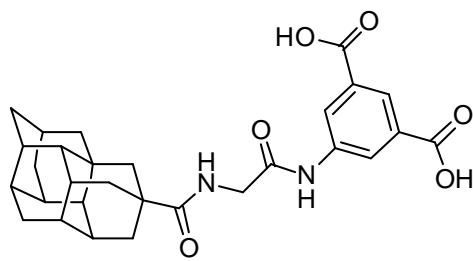


¹H-NMR of compound **9c** in DMSO-*d*6

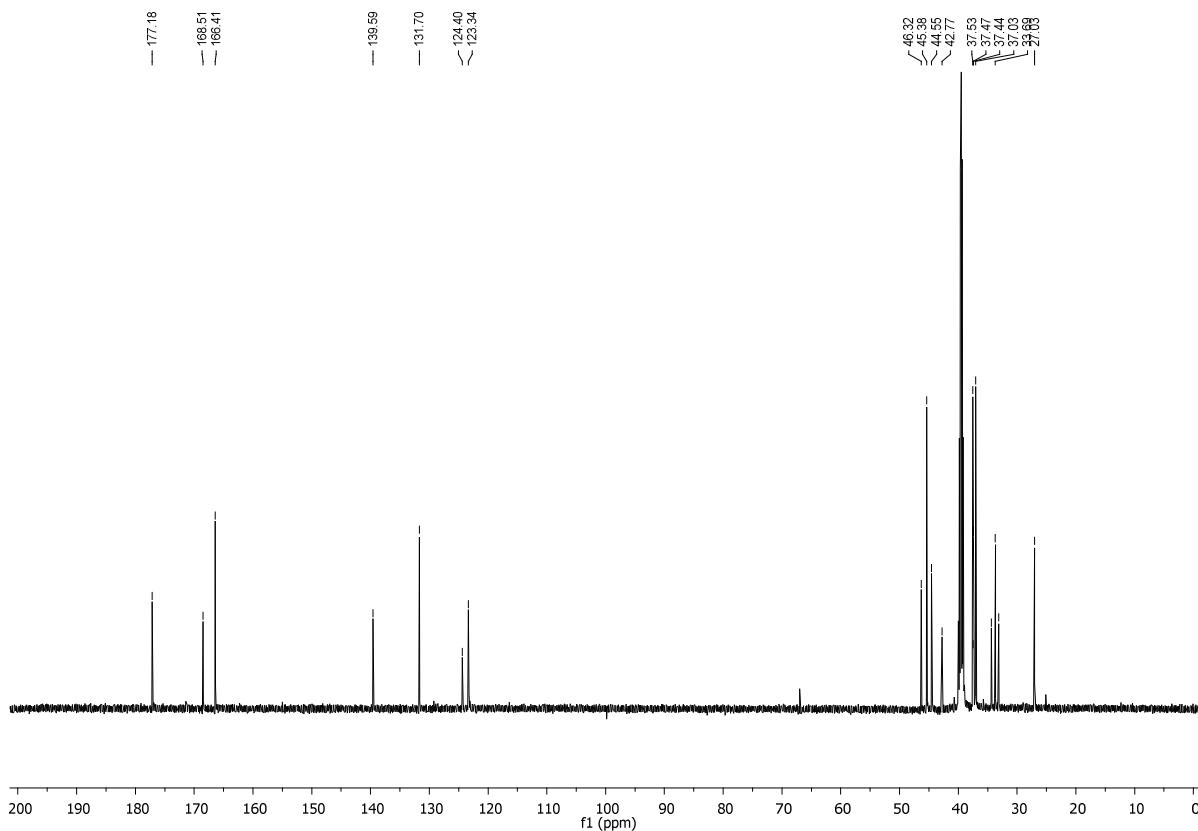


¹³C-NMR of compound **9c** in DMSO-*d*6

Electronic Supplementary Information: Nanodiamonds in Sugar Rings



¹H-NMR of compound **10c** in DMSO-*d*6

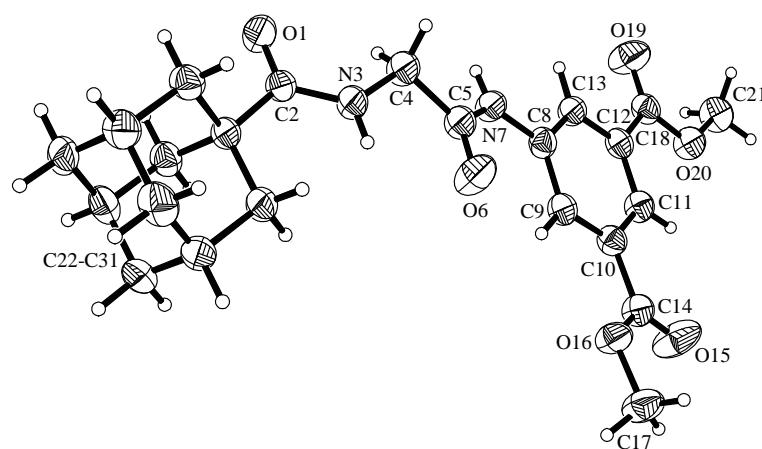


¹³C-NMR of compound **10c** in DMSO-*d*6

4. X-Ray data

Data sets were collected with a Nonius KappaCCD diffractometer. Programs used: data collection COLLECT (Nonius B.V., 1998), data reduction Denzo-SMN (Z. Otwinowski, W. Minor, *Methods in Enzymology*, **1997**, 276, 307-326), absorption correction SORTAV (R.H. Blessing, *Acta Cryst.* **1995**, A51, 33-37; R.H. Blessing, *J. Appl. Cryst.* **1997**, 30, 421-426), structure solution SHELXS-97 (G.M. Sheldrick, *Acta Cryst.* **1990**, A46, 467-473), structure refinement SHELXL-97 (G.M. Sheldrick, *Acta Cryst.* **2008**, A64, 112-122), graphics XP (BrukerAXS, 2000). Graphics show the thermal ellipsoids with 50 % probability, *R* values are given for the observed reflections, *wR*² values for all reflections.

X-Ray Structure of 7b



Crystal data for (**7b**) C₂₃H₂₈N₂O₆, *M* = 428.47, monoclinic, *P*2₁/n (No. 14), *a* = 9.7862(3), *b* = 11.6935(4), *c* = 18.1990(9) Å, β = 97.545(1)°, *V* = 2064.57(14) Å³, *D*_c = 1.378 g cm⁻³, μ = 0.100 mm⁻¹, *F*(000) = 912, *Z* = 4, λ = 0.71073 Å, *T* = 223(2) K, 12978 reflections collected (±*h*, ±*k*, ±*l*), [(sinθ)/λ] = 0.59 Å⁻¹, 3543 independent (*R*_{int} = 0.053), and 2721 observed reflections [*I* ≥ 2σ(*I*)], 288 refined parameters, *R* = 0.061, *wR*² = 0.154, GoF = 1.062.

Bond lengths of 7b

O(1)-C(2)	1.232(3)
C(2)-N(3)	1.328(3)
C(2)-C(22)	1.526(3)
N(3)-C(4)	1.446(3)
N(3)-H(3)	0.85(3)
C(4)-C(5)	1.515(4)
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(5)-O(6)	1.215(3)
C(5)-N(7)	1.353(3)
N(7)-C(8)	1.412(3)
N(7)-H(7)	0.85(3)
C(8)-C(9)	1.385(4)
C(8)-C(13)	1.386(4)
C(9)-C(10)	1.387(4)
C(9)-H(9)	0.9400
C(10)-C(11)	1.395(4)
C(10)-C(14)	1.486(4)
C(11)-C(12)	1.380(4)
C(11)-H(11)	0.9400
C(12)-C(13)	1.389(4)
C(12)-C(18)	1.493(4)
C(13)-H(13)	0.9400

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

C(14)-O(15)	1.194(3)
C(14)-O(16)	1.333(3)
O(16)-C(17)	1.438(3)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(17)-H(17C)	0.9700
C(18)-O(19)	1.197(3)
C(18)-O(20)	1.332(3)
O(20)-C(21)	1.438(3)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(21)-H(21C)	0.9700
C(22)-C(23)	1.537(3)
C(22)-C(31)	1.538(3)
C(22)-C(29)	1.543(4)
C(23)-C(24)	1.538(3)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(24)-C(30)	1.522(4)
C(24)-C(25)	1.527(4)
C(24)-H(24)	0.9900
C(25)-C(26)	1.526(4)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(26)-C(27)	1.527(4)
C(26)-C(31)	1.532(4)
C(26)-H(26)	0.9900
C(27)-C(28)	1.523(4)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(28)-C(30)	1.523(4)
C(28)-C(29)	1.525(4)
C(28)-H(28)	0.9900
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
O(1)-C(2)-N(3)	120.7(2)
O(1)-C(2)-C(22)	120.9(2)
N(3)-C(2)-C(22)	118.4(2)
C(2)-N(3)-C(4)	122.1(2)
C(2)-N(3)-H(3)	120(2)
C(4)-N(3)-H(3)	116(2)
N(3)-C(4)-C(5)	109.6(2)
N(3)-C(4)-H(4A)	109.7
C(5)-C(4)-H(4A)	109.7
N(3)-C(4)-H(4B)	109.7
C(5)-C(4)-H(4B)	109.7
H(4A)-C(4)-H(4B)	108.2
O(6)-C(5)-N(7)	124.9(3)
O(6)-C(5)-C(4)	121.1(2)
N(7)-C(5)-C(4)	114.0(2)
C(5)-N(7)-C(8)	127.7(2)
C(5)-N(7)-H(7)	117(2)
C(8)-N(7)-H(7)	115(2)
C(9)-C(8)-C(13)	119.5(2)
C(9)-C(8)-N(7)	122.7(2)
C(13)-C(8)-N(7)	117.8(2)
C(8)-C(9)-C(10)	120.1(2)
C(8)-C(9)-H(9)	120.0
C(10)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	120.3(2)
C(9)-C(10)-C(14)	122.1(2)
C(11)-C(10)-C(14)	117.6(2)
C(12)-C(11)-C(10)	119.5(2)
C(12)-C(11)-H(11)	120.2
C(10)-C(11)-H(11)	120.2

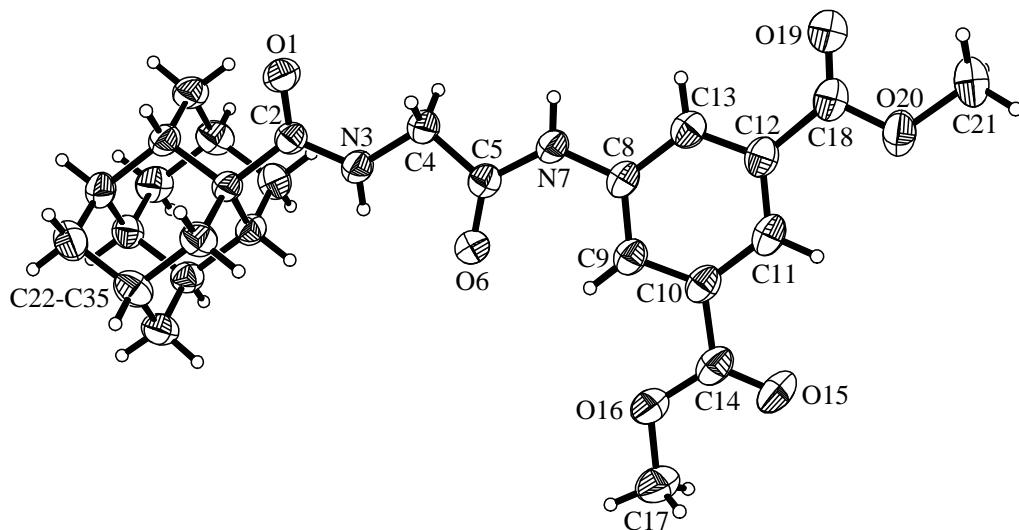
Electronic Supplementary Information: Nanodiamonds in Sugar Rings

C(11)-C(12)-C(13)	120.0(2)
C(11)-C(12)-C(18)	121.3(2)
C(13)-C(12)-C(18)	118.6(2)
C(8)-C(13)-C(12)	120.6(2)
C(8)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
O(15)-C(14)-O(16)	123.3(3)
O(15)-C(14)-C(10)	124.3(3)
O(16)-C(14)-C(10)	112.4(2)
C(14)-O(16)-C(17)	116.2(2)
O(16)-C(17)-H(17A)	109.5
O(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(19)-C(18)-O(20)	123.1(2)
O(19)-C(18)-C(12)	124.7(2)
O(20)-C(18)-C(12)	112.2(2)
C(18)-O(20)-C(21)	116.5(2)
O(20)-C(21)-H(21A)	109.5
O(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(2)-C(22)-C(23)	114.1(2)
C(2)-C(22)-C(31)	108.9(2)
C(23)-C(22)-C(31)	108.9(2)
C(2)-C(22)-C(29)	107.5(2)
C(23)-C(22)-C(29)	108.6(2)
C(31)-C(22)-C(29)	108.8(2)
C(22)-C(23)-C(24)	109.7(2)
C(22)-C(23)-H(23A)	109.7
C(24)-C(23)-H(23A)	109.7
C(22)-C(23)-H(23B)	109.7
C(24)-C(23)-H(23B)	109.7
H(23A)-C(23)-H(23B)	108.2
C(30)-C(24)-C(25)	109.9(2)
C(30)-C(24)-C(23)	109.6(2)
C(25)-C(24)-C(23)	109.3(2)
C(30)-C(24)-H(24)	109.3
C(25)-C(24)-H(24)	109.3
C(23)-C(24)-H(24)	109.3
C(26)-C(25)-C(24)	109.7(2)
C(26)-C(25)-H(25A)	109.7
C(24)-C(25)-H(25A)	109.7
C(26)-C(25)-H(25B)	109.7
C(24)-C(25)-H(25B)	109.7
H(25A)-C(25)-H(25B)	108.2
C(25)-C(26)-C(27)	108.9(2)
C(25)-C(26)-C(31)	109.7(2)
C(27)-C(26)-C(31)	109.7(2)
C(25)-C(26)-H(26)	109.5
C(27)-C(26)-H(26)	109.5
C(31)-C(26)-H(26)	109.5
C(28)-C(27)-C(26)	109.8(2)
C(28)-C(27)-H(27A)	109.7
C(26)-C(27)-H(27A)	109.7
C(28)-C(27)-H(27B)	109.7
C(26)-C(27)-H(27B)	109.7
H(27A)-C(27)-H(27B)	108.2
C(30)-C(28)-C(27)	110.3(2)
C(30)-C(28)-C(29)	109.3(2)
C(27)-C(28)-C(29)	108.9(2)
C(30)-C(28)-H(28)	109.5
C(27)-C(28)-H(28)	109.5
C(29)-C(28)-H(28)	109.5
C(28)-C(29)-C(22)	110.4(2)

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C(28)-C(29)-H(29A)	109.6
C(22)-C(29)-H(29A)	109.6
C(28)-C(29)-H(29B)	109.6
C(22)-C(29)-H(29B)	109.6
H(29A)-C(29)-H(29B)	108.1
C(24)-C(30)-C(28)	109.3(2)
C(24)-C(30)-H(30A)	109.8
C(28)-C(30)-H(30A)	109.8
C(24)-C(30)-H(30B)	109.8
C(28)-C(30)-H(30B)	109.8
H(30A)-C(30)-H(30B)	108.3
C(26)-C(31)-C(22)	109.7(2)
C(26)-C(31)-H(31A)	109.7
C(22)-C(31)-H(31A)	109.7
C(26)-C(31)-H(31B)	109.7
C(22)-C(31)-H(31B)	109.7
H(31A)-C(31)-H(31B)	108.2

X-Ray Structure of 8b



Crystal data for **(8b)** $C_{27}H_{32}N_2O_6$, $M = 480.55$, triclinic, $P\bar{1}$ bar (No. 2), $a = 8.9831(1)$, $b = 11.8982(1)$, $c = 13.1146(1)$ Å, $\alpha = 106.512(1)$, $\beta = 109.880(1)$, $\gamma = 101.331(1)$ °, $V = 1195.17(2)$ Å³, $D_c = 1.335$ g cm⁻³, $\mu = 0.773$ mm⁻¹, $F(000) = 512$, $Z = 2$, $\lambda = 1.54178$ Å, $T = 223(2)$ K, 13076 reflections collected ($\pm h$, $\pm k$, $\pm l$), $[(\sin\theta)/\lambda] = 0.60$ Å⁻¹, 3965 independent ($R_{\text{int}} = 0.044$), and 3347 observed reflections [$I \geq 2\sigma(I)$], 324 refined parameters, $R = 0.049$, $wR^2 = 0.146$, $\text{GoF} = 1.012$.

Bond lengths of 8b

O(1)-C(2)	1.261(2)
C(2)-N(3)	1.353(2)
C(2)-C(22)	1.637(2)
N(3)-C(4)	1.541(2)
N(3)-H(3)	0.86(2)
C(4)-C(5)	1.513(2)
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(5)-O(6)	1.266(2)
C(5)-N(7)	1.441(2)
N(7)-C(8)	1.429(2)
N(7)-H(7)	0.90(2)
C(8)-C(9)	1.412(3)
C(8)-C(13)	1.490(3)
C(9)-C(10)	1.413(2)

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C(9)-H(9)	0.9400
C(10)-C(11)	1.487(3)
C(10)-C(14)	1.510(3)
C(11)-C(12)	1.405(3)
C(11)-H(11)	0.9400
C(12)-C(13)	1.408(3)
C(12)-C(18)	1.591(3)
C(13)-H(13)	0.9400
C(14)-O(15)	1.220(2)
C(14)-O(16)	1.424(2)
O(16)-C(17)	1.474(3)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(17)-H(17C)	0.9700
C(18)-O(19)	1.218(3)
C(18)-O(20)	1.352(2)
O(20)-C(21)	1.536(2)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(21)-H(21C)	0.9700
C(22)-C(23)	1.511(2)
C(22)-C(35)	1.542(2)
C(22)-C(31)	1.543(2)
C(23)-C(24)	1.639(3)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(24)-C(25)	1.521(3)
C(24)-C(33)	1.526(3)
C(24)-H(24)	0.9900
C(25)-C(26)	1.485(3)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(26)-C(27)	1.533(2)
C(26)-C(35)	1.655(2)
C(26)-H(26)	0.9900
C(27)-C(28)	1.488(3)
C(27)-C(32)	1.530(3)
C(27)-H(27)	0.9900
C(28)-C(29)	1.643(3)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(29)-C(34)	1.528(3)
C(29)-C(30)	1.529(3)
C(29)-H(29)	0.9900
C(30)-C(31)	1.486(3)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(31)-C(32)	1.654(2)
C(31)-H(31)	0.9900
C(32)-C(33)	1.487(3)
C(32)-H(32)	0.9900
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(34)-C(35)	1.488(3)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(35)-H(35)	0.9900
O(1)-C(2)-N(3)	117.43(15)
O(1)-C(2)-C(22)	124.20(14)
N(3)-C(2)-C(22)	118.28(15)
C(2)-N(3)-C(4)	123.11(15)
C(2)-N(3)-H(3)	118.7(14)
C(4)-N(3)-H(3)	118.1(14)
C(5)-C(4)-N(3)	109.44(14)
C(5)-C(4)-H(4A)	109.8
N(3)-C(4)-H(4A)	109.8
C(5)-C(4)-H(4B)	109.8
N(3)-C(4)-H(4B)	109.8
H(4A)-C(4)-H(4B)	108.2

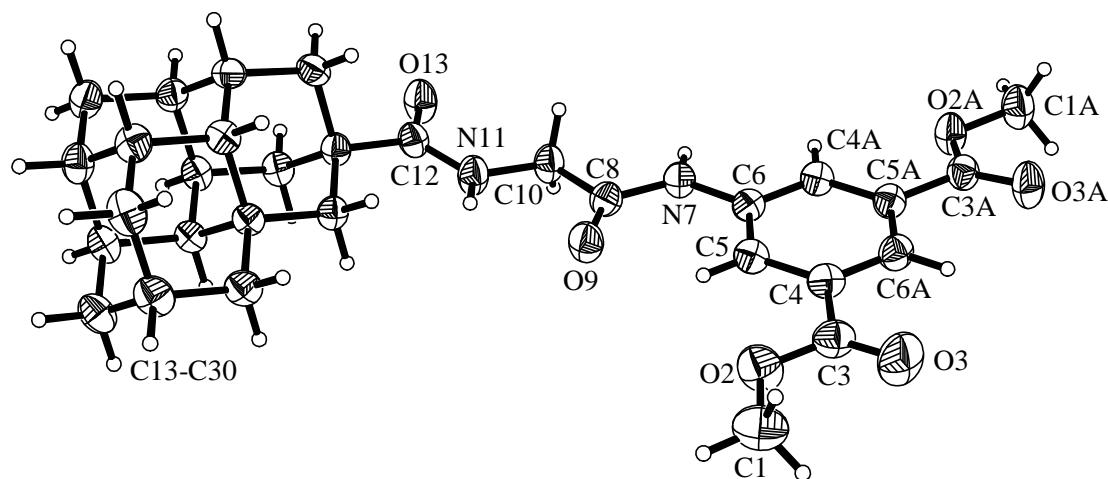
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O(6)-C(5)-N(7)	128.47(15)
O(6)-C(5)-C(4)	118.66(15)
N(7)-C(5)-C(4)	112.86(15)
C(8)-N(7)-C(5)	129.11(15)
C(8)-N(7)-H(7)	111.8(13)
C(5)-N(7)-H(7)	119.1(13)
C(9)-C(8)-N(7)	120.02(16)
C(9)-C(8)-C(13)	121.54(15)
N(7)-C(8)-C(13)	118.44(15)
C(8)-C(9)-C(10)	115.43(17)
C(8)-C(9)-H(9)	122.3
C(10)-C(9)-H(9)	122.3
C(9)-C(10)-C(11)	122.89(17)
C(9)-C(10)-C(14)	117.82(17)
C(11)-C(10)-C(14)	119.26(16)
C(12)-C(11)-C(10)	121.47(16)
C(12)-C(11)-H(11)	119.3
C(10)-C(11)-H(11)	119.3
C(11)-C(12)-C(13)	116.00(18)
C(11)-C(12)-C(18)	124.09(16)
C(13)-C(12)-C(18)	119.89(17)
C(12)-C(13)-C(8)	122.67(17)
C(12)-C(13)-H(13)	118.7
C(8)-C(13)-H(13)	118.7
O(15)-C(14)-O(16)	124.61(19)
O(15)-C(14)-C(10)	120.24(19)
O(16)-C(14)-C(10)	115.14(15)
C(14)-O(16)-C(17)	117.75(15)
O(16)-C(17)-H(17A)	109.5
O(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(19)-C(18)-O(20)	119.34(19)
O(19)-C(18)-C(12)	126.64(17)
O(20)-C(18)-C(12)	114.02(17)
C(18)-O(20)-C(21)	118.11(17)
O(20)-C(21)-H(21A)	109.5
O(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-C(35)	106.77(14)
C(23)-C(22)-C(31)	107.03(14)
C(35)-C(22)-C(31)	108.07(14)
C(23)-C(22)-C(2)	109.06(13)
C(35)-C(22)-C(2)	114.45(13)
C(31)-C(22)-C(2)	111.12(13)
C(22)-C(23)-C(24)	113.05(14)
C(22)-C(23)-H(23A)	109.0
C(24)-C(23)-H(23A)	109.0
C(22)-C(23)-H(23B)	109.0
C(24)-C(23)-H(23B)	109.0
H(23A)-C(23)-H(23B)	107.8
C(25)-C(24)-C(33)	110.07(17)
C(25)-C(24)-C(23)	110.83(16)
C(33)-C(24)-C(23)	109.76(16)
C(25)-C(24)-H(24)	108.7
C(33)-C(24)-H(24)	108.7
C(23)-C(24)-H(24)	108.7
C(26)-C(25)-C(24)	106.84(15)
C(26)-C(25)-H(25A)	110.4
C(24)-C(25)-H(25A)	110.4
C(26)-C(25)-H(25B)	110.4
C(24)-C(25)-H(25B)	110.4
H(25A)-C(25)-H(25B)	108.6
C(25)-C(26)-C(27)	107.97(15)

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C(25)-C(26)-C(35)	113.28(14)
C(27)-C(26)-C(35)	109.52(14)
C(25)-C(26)-H(26)	108.7
C(27)-C(26)-H(26)	108.7
C(35)-C(26)-H(26)	108.7
C(28)-C(27)-C(32)	108.36(16)
C(28)-C(27)-C(26)	108.19(16)
C(32)-C(27)-C(26)	108.77(14)
C(28)-C(27)-H(27)	110.5
C(32)-C(27)-H(27)	110.5
C(26)-C(27)-H(27)	110.5
C(27)-C(28)-C(29)	111.56(15)
C(27)-C(28)-H(28A)	109.3
C(29)-C(28)-H(28A)	109.3
C(27)-C(28)-H(28B)	109.3
C(29)-C(28)-H(28B)	109.3
H(28A)-C(28)-H(28B)	108.0
C(34)-C(29)-C(30)	109.95(15)
C(34)-C(29)-C(28)	110.13(16)
C(30)-C(29)-C(28)	110.46(16)
C(34)-C(29)-H(29)	108.8
C(30)-C(29)-H(29)	108.8
C(28)-C(29)-H(29)	108.8
C(31)-C(30)-C(29)	107.08(15)
C(31)-C(30)-H(30A)	110.3
C(29)-C(30)-H(30A)	110.3
C(31)-C(30)-H(30B)	110.3
C(29)-C(30)-H(30B)	110.3
H(30A)-C(30)-H(30B)	108.6
C(30)-C(31)-C(22)	108.47(15)
C(30)-C(31)-C(32)	112.21(15)
C(22)-C(31)-C(32)	109.89(14)
C(30)-C(31)-H(31)	108.7
C(22)-C(31)-H(31)	108.7
C(32)-C(31)-H(31)	108.7
C(33)-C(32)-C(27)	107.91(16)
C(33)-C(32)-C(31)	113.21(15)
C(27)-C(32)-C(31)	109.78(14)
C(33)-C(32)-H(32)	108.6
C(27)-C(32)-H(32)	108.6
C(31)-C(32)-H(32)	108.6
C(32)-C(33)-C(24)	107.04(16)
C(32)-C(33)-H(33A)	110.3
C(24)-C(33)-H(33A)	110.3
C(32)-C(33)-H(33B)	110.3
C(24)-C(33)-H(33B)	110.3
H(33A)-C(33)-H(33B)	108.6
C(35)-C(34)-C(29)	107.52(15)
C(35)-C(34)-H(34A)	110.2
C(29)-C(34)-H(34A)	110.2
C(35)-C(34)-H(34B)	110.2
C(29)-C(34)-H(34B)	110.2
H(34A)-C(34)-H(34B)	108.5
C(34)-C(35)-C(22)	107.77(15)
C(34)-C(35)-C(26)	112.22(14)
C(22)-C(35)-C(26)	110.27(13)
C(34)-C(35)-H(35)	108.8
C(22)-C(35)-H(35)	108.8
C(26)-C(35)-H(35)	108.8

X-Ray Structure of **10b**



Crystal data for (**10b**) $C_{31}H_{36}N_2O_6$, $M = 532.62$, triclinic, $P\bar{1}$ bar (No. 2), $a = 8.8685(2)$, $b = 11.1349(2)$, $c = 14.0791(3)$ Å, $\alpha = 94.026(1)$, $\beta = 96.563(1)$, $\gamma = 109.563(1)$ °, $V = 1292.70(5)$ Å³, $D_c = 1.368$ g cm⁻³, $\mu = 0.095$ mm⁻¹, $F(000) = 568$, $Z = 2$, $\lambda = 0.71073$ Å, $T = 223(2)$ K, 11599 reflections collected ($\pm h$, $\pm k$, $\pm l$), $[(\sin\theta)/\lambda] = 0.66$ Å⁻¹, 5972 independent ($R_{\text{int}} = 0.045$), and 4959 observed reflections [$I \geq 2\sigma(I)$], 360 refined parameters, $R = 0.060$, $wR^2 = 0.157$, $\text{GoF} = 1.023$.

Bond lengths of **10 b**

C(1)-O(2)	1.447(2)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(1)-H(1C)	0.9700
O(2)-C(3)	1.330(3)
C(3)-O(3)	1.200(3)
C(3)-C(4)	1.493(3)
C(4)-C(6A)	1.385(3)
C(4)-C(5)	1.393(3)
C(5)-C(6)	1.398(2)
C(5)-H(5)	0.9400
C(6)-C(4A)	1.395(3)
C(6)-N(7)	1.411(2)
C(1A)-O(2A)	1.447(2)
C(1A)-H(1A1)	0.9700
C(1A)-H(1A2)	0.9700
C(1A)-H(1A3)	0.9700
O(2A)-C(3A)	1.338(2)
C(3A)-O(3A)	1.202(2)
C(3A)-C(5A)	1.488(3)
C(4A)-C(5A)	1.392(2)
C(4A)-H(4A)	0.9400
C(5A)-C(6A)	1.391(3)
C(6A)-H(6A)	0.9400
N(7)-C(8)	1.358(2)
N(7)-H(7)	0.86(2)
C(8)-O(9)	1.221(2)
C(8)-C(10)	1.517(3)
C(10)-N(11)	1.447(2)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
N(11)-C(12)	1.328(2)
N(11)-H(11)	0.84(3)
C(12)-O(13)	1.237(2)

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C(12)-C(13)	1.523(2)
C(13)-C(14)	1.536(2)
C(13)-C(15)	1.538(2)
C(13)-C(16)	1.542(3)
C(14)-C(19)	1.531(2)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(15)-C(21)	1.528(2)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(16)-C(17)	1.531(2)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(17)-C(18)	1.533(2)
C(17)-C(20)	1.539(3)
C(17)-H(17)	0.9900
C(18)-C(26)	1.542(2)
C(18)-C(19)	1.547(2)
C(18)-H(18)	0.9900
C(19)-C(22)	1.532(2)
C(19)-C(23)	1.541(2)
C(20)-C(27)	1.533(2)
C(20)-C(21)	1.537(3)
C(20)-H(20)	0.9900
C(21)-C(23)	1.532(2)
C(21)-H(21)	0.9900
C(22)-C(24)	1.529(3)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(23)-C(29)	1.540(2)
C(23)-H(23)	0.9900
C(24)-C(30)	1.532(3)
C(24)-C(25)	1.532(3)
C(24)-H(24)	0.9900
C(25)-C(26)	1.528(3)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(26)-C(28)	1.535(3)
C(26)-H(26)	0.9900
C(27)-C(28)	1.529(3)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(28)-C(29)	1.535(3)
C(28)-H(28)	0.9900
C(29)-C(30)	1.534(3)
C(29)-H(29)	0.9900
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
O(2)-C(1)-H(1A)	109.5
O(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(3)-O(2)-C(1)	116.43(18)
O(3)-C(3)-O(2)	123.12(19)
O(3)-C(3)-C(4)	123.9(2)
O(2)-C(3)-C(4)	113.02(17)
C(6A)-C(4)-C(5)	120.78(17)
C(6A)-C(4)-C(3)	118.07(17)
C(5)-C(4)-C(3)	121.12(18)
C(4)-C(5)-C(6)	119.59(17)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-H(5)	120.2
C(4A)-C(6)-C(5)	119.72(16)
C(4A)-C(6)-N(7)	117.04(16)
C(5)-C(6)-N(7)	123.24(16)
O(2A)-C(1A)-H(1A1)	109.5
O(2A)-C(1A)-H(1A2)	109.5

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H(1A1)-C(1A)-H(1A2)	109.5
O(2A)-C(1A)-H(1A3)	109.5
H(1A1)-C(1A)-H(1A3)	109.5
H(1A2)-C(1A)-H(1A3)	109.5
C(3A)-O(2A)-C(1A)	115.06(15)
O(3A)-C(3A)-O(2A)	123.12(18)
O(3A)-C(3A)-C(5A)	123.42(18)
O(2A)-C(3A)-C(5A)	113.45(15)
C(5A)-C(4A)-C(6)	120.01(17)
C(5A)-C(4A)-H(4A)	120.0
C(6)-C(4A)-H(4A)	120.0
C(6A)-C(5A)-C(4A)	120.29(18)
C(6A)-C(5A)-C(3A)	117.44(16)
C(4A)-C(5A)-C(3A)	122.24(17)
C(4)-C(6A)-C(5A)	119.60(17)
C(4)-C(6A)-H(6A)	120.2
C(5A)-C(6A)-H(6A)	120.2
C(8)-N(7)-C(6)	127.28(16)
C(8)-N(7)-H(7)	116.1(15)
C(6)-N(7)-H(7)	116.3(15)
O(9)-C(8)-N(7)	125.24(17)
O(9)-C(8)-C(10)	121.52(17)
N(7)-C(8)-C(10)	113.23(16)
N(11)-C(10)-C(8)	108.17(15)
N(11)-C(10)-H(10A)	110.1
C(8)-C(10)-H(10A)	110.1
N(11)-C(10)-H(10B)	110.1
C(8)-C(10)-H(10B)	110.1
H(10A)-C(10)-H(10B)	108.4
C(12)-N(11)-C(10)	122.87(16)
C(12)-N(11)-H(11)	122.3(17)
C(10)-N(11)-H(11)	114.4(17)
O(13)-C(12)-N(11)	120.99(17)
O(13)-C(12)-C(13)	121.51(16)
N(11)-C(12)-C(13)	117.49(16)
C(12)-C(13)-C(14)	114.37(14)
C(12)-C(13)-C(15)	108.89(14)
C(14)-C(13)-C(15)	108.76(14)
C(12)-C(13)-C(16)	107.45(14)
C(14)-C(13)-C(16)	108.27(14)
C(15)-C(13)-C(16)	108.98(14)
C(19)-C(14)-C(13)	111.19(14)
C(19)-C(14)-H(14A)	109.4
C(13)-C(14)-H(14A)	109.4
C(19)-C(14)-H(14B)	109.4
C(13)-C(14)-H(14B)	109.4
H(14A)-C(14)-H(14B)	108.0
C(21)-C(15)-C(13)	109.92(14)
C(21)-C(15)-H(15A)	109.7
C(13)-C(15)-H(15A)	109.7
C(21)-C(15)-H(15B)	109.7
C(13)-C(15)-H(15B)	109.7
H(15A)-C(15)-H(15B)	108.2
C(17)-C(16)-C(13)	109.94(14)
C(17)-C(16)-H(16A)	109.7
C(13)-C(16)-H(16A)	109.7
C(17)-C(16)-H(16B)	109.7
C(13)-C(16)-H(16B)	109.7
H(16A)-C(16)-H(16B)	108.2
C(16)-C(17)-C(18)	110.25(14)
C(16)-C(17)-C(20)	110.50(15)
C(18)-C(17)-C(20)	109.11(14)
C(16)-C(17)-H(17)	109.0
C(18)-C(17)-H(17)	109.0
C(20)-C(17)-H(17)	109.0
C(17)-C(18)-C(26)	111.41(15)
C(17)-C(18)-C(19)	109.18(14)
C(26)-C(18)-C(19)	109.10(14)
C(17)-C(18)-H(18)	109.0

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C(26)-C(18)-H(18)	109.0
C(19)-C(18)-H(18)	109.0
C(14)-C(19)-C(22)	110.72(14)
C(14)-C(19)-C(23)	109.51(13)
C(22)-C(19)-C(23)	109.37(14)
C(14)-C(19)-C(18)	109.62(14)
C(22)-C(19)-C(18)	109.95(14)
C(23)-C(19)-C(18)	107.62(14)
C(27)-C(20)-C(21)	109.71(15)
C(27)-C(20)-C(17)	110.40(15)
C(21)-C(20)-C(17)	108.13(14)
C(27)-C(20)-H(20)	109.5
C(21)-C(20)-H(20)	109.5
C(17)-C(20)-H(20)	109.5
C(15)-C(21)-C(23)	110.34(14)
C(15)-C(21)-C(20)	110.59(15)
C(23)-C(21)-C(20)	108.76(14)
C(15)-C(21)-H(21)	109.0
C(23)-C(21)-H(21)	109.0
C(20)-C(21)-H(21)	109.0
C(24)-C(22)-C(19)	110.57(15)
C(24)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22A)	109.5
C(24)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	108.1
C(21)-C(23)-C(29)	111.28(14)
C(21)-C(23)-C(19)	109.68(14)
C(29)-C(23)-C(19)	109.82(13)
C(21)-C(23)-H(23)	108.7
C(29)-C(23)-H(23)	108.7
C(19)-C(23)-H(23)	108.7
C(22)-C(24)-C(30)	109.10(15)
C(22)-C(24)-C(25)	109.41(16)
C(30)-C(24)-C(25)	109.08(17)
C(22)-C(24)-H(24)	109.7
C(30)-C(24)-H(24)	109.7
C(25)-C(24)-H(24)	109.7
C(26)-C(25)-C(24)	109.99(15)
C(26)-C(25)-H(25A)	109.7
C(24)-C(25)-H(25A)	109.7
C(26)-C(25)-H(25B)	109.7
C(24)-C(25)-H(25B)	109.7
H(25A)-C(25)-H(25B)	108.2
C(25)-C(26)-C(28)	110.38(16)
C(25)-C(26)-C(18)	110.11(16)
C(28)-C(26)-C(18)	108.79(14)
C(25)-C(26)-H(26)	109.2
C(28)-C(26)-H(26)	109.2
C(18)-C(26)-H(26)	109.2
C(28)-C(27)-C(20)	109.89(15)
C(28)-C(27)-H(27A)	109.7
C(20)-C(27)-H(27A)	109.7
C(28)-C(27)-H(27B)	109.7
C(20)-C(27)-H(27B)	109.7
H(27A)-C(27)-H(27B)	108.2
C(27)-C(28)-C(29)	109.88(15)
C(27)-C(28)-C(26)	110.61(16)
C(29)-C(28)-C(26)	108.60(15)
C(27)-C(28)-H(28)	109.2
C(29)-C(28)-H(28)	109.2
C(26)-C(28)-H(28)	109.2
C(30)-C(29)-C(28)	110.74(15)
C(30)-C(29)-C(23)	109.78(15)
C(28)-C(29)-C(23)	108.35(15)
C(30)-C(29)-H(29)	109.3
C(28)-C(29)-H(29)	109.3
C(23)-C(29)-H(29)	109.3
C(24)-C(30)-C(29)	109.64(16)

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C(24)-C(30)-H(30A)	109.7
C(29)-C(30)-H(30A)	109.7
C(24)-C(30)-H(30B)	109.7
C(29)-C(30)-H(30B)	109.7
H(30A)-C(30)-H(30B)	108.2

5. Computational details

Nr	ND	Guest	Host	BE	DE ^{CD}	DE ND	RMSD ^{CD}	RMSD ND	Rp	Pept	Tilt
				(kJ/mol)	(kJ/mol)	(kJ/mol)	(Å)	(Å)	(Å)	(ψ)	(θ)
A	1-Adamantane	(7a)	β-CD	-100	63	20	0.93	0.42	1.62	-	21
B		(7a)	γ-CD	-69	6	25	0.69	0.62	0.3	-	106
C		(7c)	β-CD	-96	111	53	0.83	2.72	1.19	80	17
D		(7c)	γ-CD	-140	6	27	0.69	2.74	0.3	70	106
E^b	1-Diamantane	(8a)	β-CD	-70	54	9	0.62	0.10	1.62	-	21
F		(8a)	γ-CD	-152	-29	13	0.65	2.61	1.23	-	7.8
G		(8c)	β-CD	-112	128	30	0.78	2.23	2.2	98	10
H		(8c)	γ-CD	-207	-1	6	1.02	3.34	2.71	63	23
I	4-Diamantane	(9a)	β-CD	-5	98	0	1.12	0.39	1.39	-	174
J		(9a)	γ-CD	-145	17	12	1.36	2.7	1.8	-	27
K		(9c)	β-CD	-42	122	24	1.11	1.85	1.2	63	174
L		(9c)	γ-CD	-179	40	35	0.94	3.86	2.8	161	30
M	9-Triamantane	(10a)	β-CD	-84	62	19	0.81	0.53	2.4	-	22
N		(10a)	γ-CD	-173	-29	2	1.19	0.5	0.6	-	27
O		(10c)	β-CD	-137	102	12	0.81	3.18	0.3	77	42
P		(10c)	γ-CD	-a-	-a-						

Table S1: The gas-phase energetics of ND•CD complexes at the B97-D3/def2-TZVPP level of theory, and the structural descriptors of ND•CD complexes that were optimized at the B973-D/def-SV(P) level of theory. Note: only the complexes listed where the primary orifice of the CD ring was penetrated by the ligands are presented here.

Density functional validation

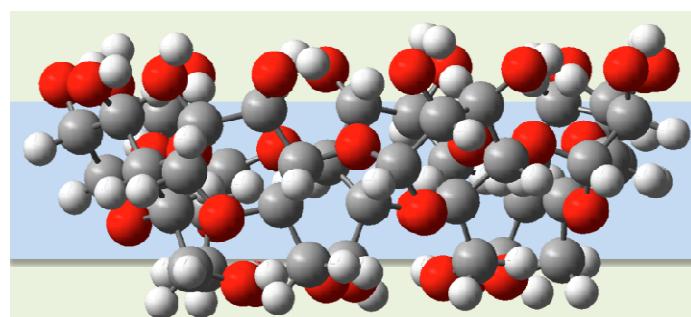


Figure S1: Side view γ -CD showing the hydrophobic blue region, and the green hydrophilic CD rim

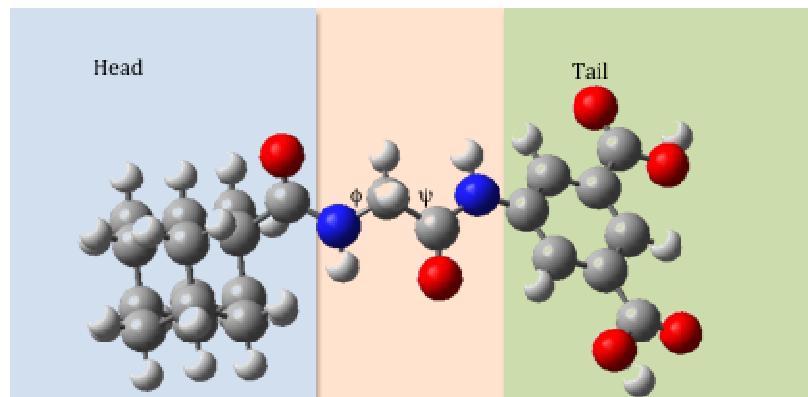


Figure S2: Blue is hydrophobic adamantane core, Green is hydrophilic substituent, and the tan is the highly flexible linker.

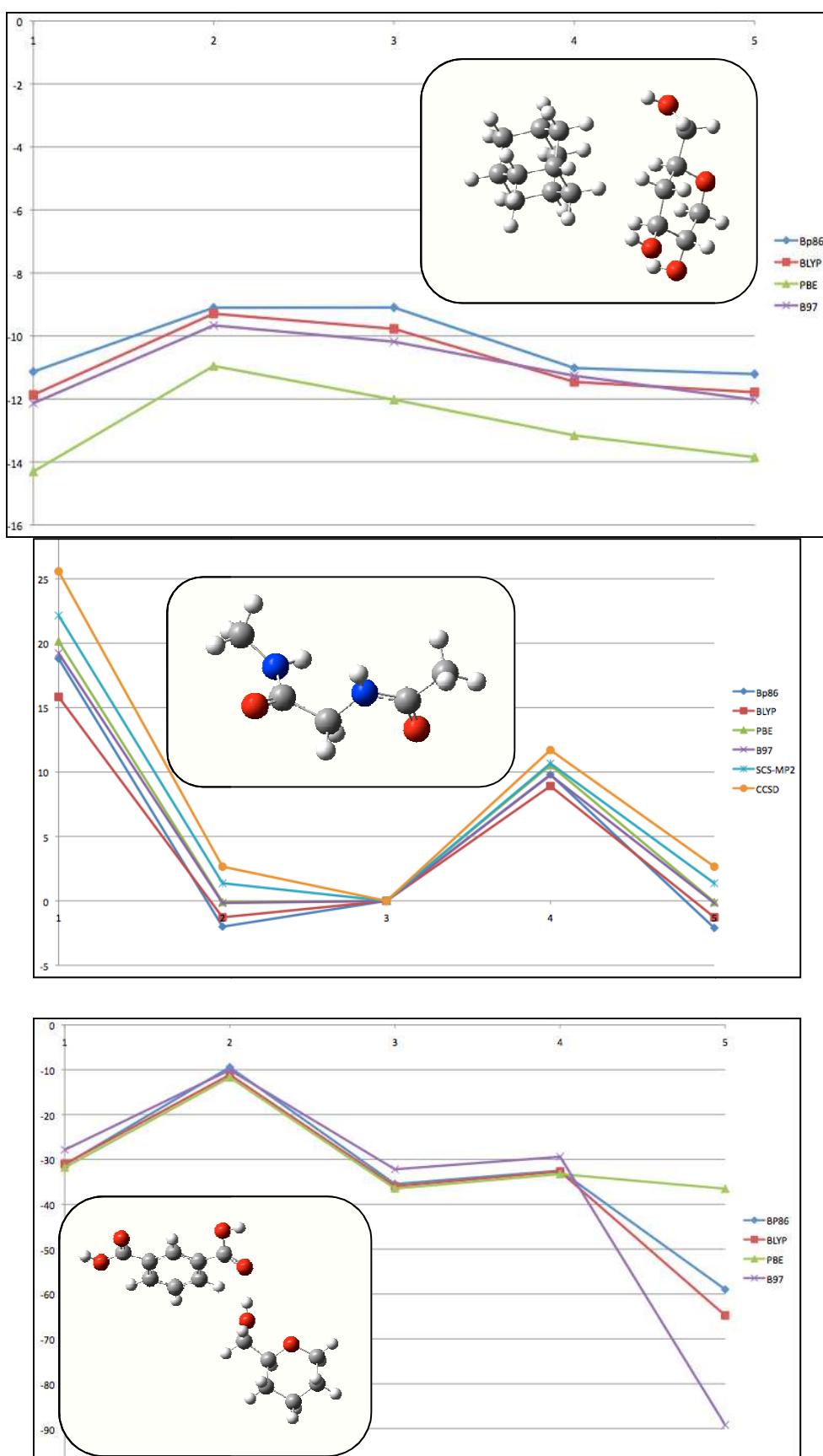


Figure S3: Interaction energies across five conformers, for three difference types of interactions. Note the values are non-CP corrected values.



Figure. S4: 7a@ β -CD (left) and 7a@ γ -CD (right).

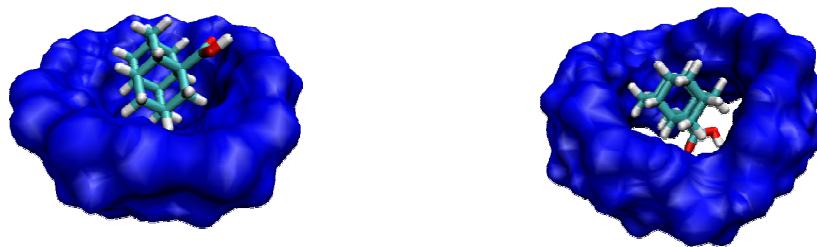


Figure. S5: 8a@ β -CD (left) and 8a@ γ -CD (right).

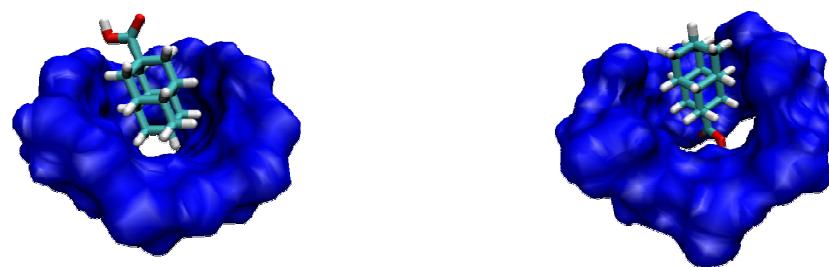


Figure. S6: 9a@ β -CD (left) and 9a@ γ -CD (right)

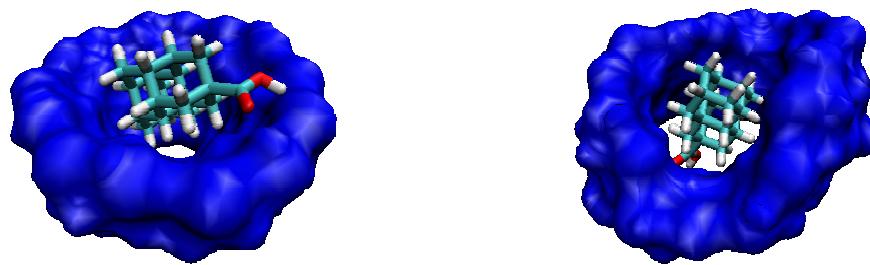


Figure. S6: 10a@ β -CD (left) and 10a@ γ -CD (right).

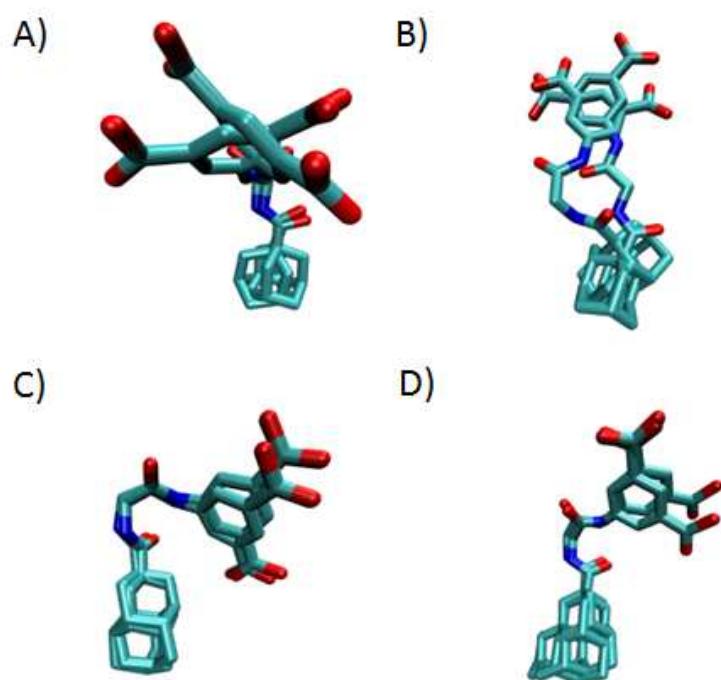


Figure S7: A. The overlaid **7c** S and P displaying the perpendicular and planar geometries. B. The overlaid **8c** S and P displaying the *cis-trans*-isomerisation. C. The overlaid **9c** S and P displaying only the *cis* isomer D. The overlaid **10C** S and P displaying similar behavior to the **9c** ligands

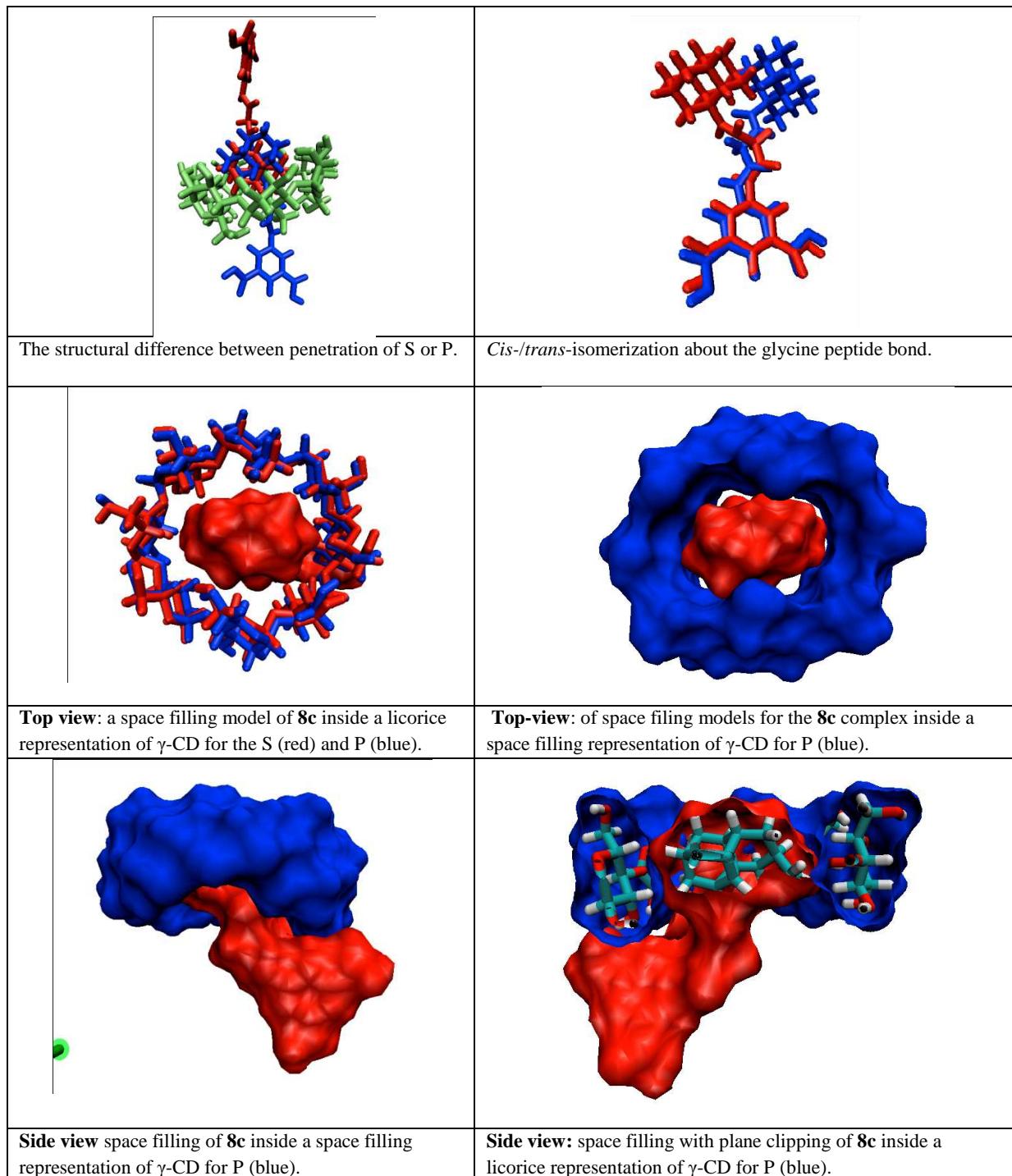


Figure S8

6. Gas phase optimized coordinates:

7a_beta-CD_P:

C	5.95283884	-2.02022284	-2.48450644	C	-0.02707301	-5.18606471	-1.35132861
C	6.85052544	-0.91148376	-1.90182507	O	-0.07584277	-3.95592885	-2.08186097
O	7.59388538	-1.34978417	-0.77850292	C	3.26408948	-5.93053807	-0.04894765
C	6.01134488	0.33385175	-1.55997431	C	4.62333260	-5.58462563	0.58718233
O	6.86246723	1.40938606	-1.18434918	O	4.66189125	-5.83175039	1.98002265
C	5.13772369	0.75847806	-2.74752644	C	4.97389536	-4.12318105	0.26530769
O	4.32027299	1.83194750	-2.30680656	O	6.27879642	-3.79684276	0.72905035
C	4.28735736	-0.46345957	-3.17326994	C	4.90857600	-3.87461647	-1.24337954
O	5.18297591	-1.53106953	-3.55924547	O	5.14442100	-2.48346968	-1.42181156
C	3.29406282	-0.22859963	-4.31420946	C	3.52209522	-4.29824489	-1.79224331
O	2.21632245	-1.17456897	-4.30983237	O	3.26629911	-5.67600812	-1.43347103
C	4.10556359	2.95788200	-3.15318786	C	3.38352669	-4.19897175	-3.31821245
C	4.70419275	4.19828877	-2.44237550	O	2.06241882	-3.84350413	-3.73486892
O	6.07952909	4.02159547	-2.21707942	H	6.57025249	-2.84545763	-2.89505616
C	3.87421605	4.50655495	-1.18275169	H	7.58249690	-0.61928501	-2.68029857
O	4.26958400	5.74721495	-0.63792293	H	7.01205136	-1.93744783	-0.24069586
C	2.37936927	4.53515122	-1.55513040	H	5.32906029	0.07068503	-0.72224564
O	1.64003069	4.73802162	-0.34339145	H	7.50278952	1.04295375	-0.53982829
C	1.91313102	3.25603140	-2.26928463	H	5.79637728	1.07865830	-3.58299348
O	2.73403548	3.09164050	-3.44225051	H	3.70204313	-0.77608053	-2.28900718
C	0.43393778	3.26701159	-2.70259450	H	3.81189754	-0.33133790	-5.28735020
O	-0.30305488	2.38160776	-1.87717088	H	2.88515657	0.79943179	-4.23006792
C	0.94760176	5.94086457	-0.18154961	H	1.73610713	-1.06845471	-3.45402111
C	1.07522834	6.39680088	1.28854218	H	4.61118582	2.81137908	-4.12841584
O	2.44824805	6.52695952	1.62239631	H	4.60482830	5.06533520	-3.12643183
C	0.36405320	5.39186789	2.19029654	H	6.21347299	3.20273554	-1.68569733
O	0.41623533	5.86238688	3.53206417	H	4.02738570	3.67055614	-0.45915311
C	-1.07993088	5.18421099	1.71975873	H	3.75367370	5.88784591	0.18767655
O	-1.60018184	4.13774294	2.55142528	H	2.21629742	5.38984082	-2.24447657
C	-1.11989399	4.79656379	0.22800237	H	2.05354326	2.38814589	-1.59726504
O	-0.42579732	5.81130427	-0.52274890	H	0.40250106	2.94654871	-3.77008814
C	-2.54301676	4.67215519	-0.35106389	H	0.02587935	4.30018838	-2.64458103
O	-2.70089793	3.53658827	-1.19619016	H	-1.21767702	2.74078775	-1.74428870
C	-2.83884280	4.25837449	3.17859659	H	1.34680693	6.72742730	-0.85187374
C	-2.69541800	3.72271113	4.62503330	H	0.55532772	7.37835472	1.37552294
O	-1.62119172	4.34410135	5.34055790	H	2.50243948	6.55672913	2.59882721
C	-2.41328134	2.21762749	4.61021885	H	0.89399568	4.42179789	2.09283072
O	-2.48133145	1.66885030	5.92213619	H	-0.01642966	5.17549389	4.08672688
C	-3.43979451	1.48378652	3.73795337	H	-1.65360464	6.12206129	1.88429283
O	-3.04608823	0.12375221	3.70596381	H	-0.60265519	3.82484271	0.10988528
C	-3.51228419	2.12730662	2.33509067	H	-2.74385944	5.59697938	-0.93297367
O	-3.85596558	3.52172138	2.51322145	H	-3.27045875	4.62136492	0.48256100
C	-4.57082648	1.52053601	1.40490518	H	-3.35344285	2.91738063	-0.77823046
O	-4.75189727	2.32578505	0.23726962	H	-3.19060140	5.31229254	3.18155055
C	-4.04676487	-0.88575324	3.74756523	H	-3.66126912	3.88507251	5.14944062
C	-3.60525328	-1.91328697	4.81134169	H	-1.90597569	5.23252105	5.62888680
O	-3.31605079	-1.31524770	6.06111284	H	-1.40829795	2.05932397	4.16931086
C	-2.41661208	-2.74469178	4.30021896	H	-1.82689426	2.15168870	6.46468503
O	-2.14125019	-3.81152876	5.20268394	H	-4.43646741	1.58669940	4.22064906
C	-2.70540354	-3.31684877	2.90927167	H	-2.52288633	2.05690419	1.84134176
O	-1.53560006	-3.99503443	2.47122703	H	-4.24646497	0.52169475	1.06265699
C	-3.06113900	-2.14237137	1.97396111	H	-5.53701550	1.41207147	1.94806040
O	-4.23334896	-1.48193363	2.49622385	H	-5.08910884	3.19264084	0.54026481
C	-3.34692469	-2.49961255	0.51384659	H	-5.02367567	-0.44403334	4.02975410
O	-3.26165579	-1.35643909	-0.32076590	H	-4.44941437	-2.61206936	4.97678220
C	-1.61267762	-5.33914423	2.02053418	H	-2.83925340	-0.46826670	5.89110831
C	-0.56486253	-6.14613551	2.81893432	H	-1.52920129	-2.07692411	4.21245003
O	-0.76708510	-6.11791006	4.21553772	H	-2.11387402	-3.41732261	6.09944834
C	0.83170673	-5.63283232	2.44063372	H	-3.56627227	-4.01662496	2.97296040
O	1.85394635	-6.37924764	3.09060141	H	-2.20646392	-1.43561381	1.98165817
C	1.02845114	-5.74000717	0.93299247	H	-4.38269297	-2.89016189	0.44361836
O	2.29050193	-5.15831394	0.62540218	H	-2.64924892	-3.30395607	0.19836248
C	-0.09139429	-4.98608967	0.18090548	H	-2.30916707	-1.22122022	-0.51877580
O	-1.38774088	-5.43923402	0.63340767	H	-2.62861605	-5.74951902	2.19198290
				H	-0.64112994	-7.20749743	2.50623280
				H	-1.06490166	-5.21429367	4.48941001

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H	0.89510372	-4.55762564	2.72164963		1	2.335431050	1.953176335	-0.569949435
H	1.55871939	-6.47706093	4.02096292		6	0.951333538	1.039751452	0.849092286
H	1.01293004	-6.81354084	0.64677550		1	1.350610848	1.630732915	1.699166270
H	0.02036698	-3.91348738	0.42061084		6	2.489990289	0.085222599	-2.616828032
H	-0.89095806	-5.82276237	-1.63648425		8	2.247184727	-0.446137877	-3.702616529
H	0.90608525	-5.71804333	-1.61921575		1	-1.671686175	-1.079412821	-1.255003341
H	0.72646281	-3.89100850	-2.69428388		1	-0.172490595	0.220942646	-2.873305671
H	3.05199782	-7.01295420	0.06416474		1	0.786167730	-1.917893622	-1.804667984
H	5.39302940	-6.22999792	0.11589322		6	1.924937431	5.664116345	-3.060645170
H	3.75079630	-5.73301497	2.34484401		6	2.740371906	4.615984218	-3.862655641
H	4.21249070	-3.46968712	0.74914084		6	3.552966504	3.730535185	-2.895150859
H	6.32765464	-4.13366405	1.64819531		6	4.352536749	4.599766909	-1.917961457
H	5.70524070	-4.47047216	-1.74028253		6	3.465897373	5.637632410	-1.214187487
H	2.76224999	-3.63918657	-1.32958784		6	4.272439962	6.604631008	-0.342661806
H	3.64536916	-5.19009606	-3.74492157		8	1.929649659	3.870126216	-4.731645278
H	4.09346540	-3.44551994	-3.70374256		8	4.411918718	2.836125434	-3.624716711
H	2.12022914	-2.91611969	-4.10032578		8	4.914151192	3.749448990	-0.925473423
C	1.18344238	-0.55567835	0.57847879		8	2.766806406	6.437783786	-2.205727394
C	2.62263529	0.00162527	0.44484649		8	5.326227025	7.235890697	-1.059355008
H	2.68734871	0.68566841	-0.42080223		6	6.271035394	3.916738524	-0.556748918
C	1.14620574	-1.55481194	1.77572320		6	7.126832986	2.865288070	-1.281988301
H	0.13062740	-1.98096047	1.88288367		6	6.629637294	1.460002131	-0.919386239
C	3.03267070	0.73281306	1.73980311		6	6.647134477	1.283237054	0.602763351
H	4.06050136	1.13266143	1.61730230		6	5.898319014	2.445438306	1.294933527
C	1.56104380	-0.82494954	3.07473434		6	6.085191943	2.429382163	2.813007241
H	1.52620826	-1.54840841	3.91725119		8	7.046471139	3.057581678	-2.700198130
C	2.99388281	-0.26213259	2.92313485		8	7.388538087	0.497848696	-1.642800559
H	3.30332060	0.24514095	3.86203495		8	5.971674538	0.073841298	0.942039127
C	2.04775536	1.89567297	1.99880076		8	6.394607770	3.721902653	0.833082288
H	2.34145098	2.45135411	2.91589989		8	7.452607878	2.453080927	3.191770223
H	2.07859278	2.61372559	1.15354804		6	6.649976254	-0.912268546	1.695495389
C	0.57750741	0.33805100	3.34625933		6	7.550457757	-1.809271794	0.819400886
H	-0.45311220	-0.05359295	3.47485171		6	6.707933143	-2.437931704	-0.291564641
H	0.85471646	0.85555633	4.29073194		6	5.525669485	-3.218607098	0.306060716
C	0.19204399	0.60887815	0.86710210		6	4.772103260	-2.363037423	1.346529563
H	0.18401913	1.31147620	0.01135854		6	3.781640520	-3.163499034	2.190562989
H	-0.83486581	0.20044691	0.97182795		8	8.644238497	-1.078082289	0.251023118
C	0.61613795	1.33268398	2.16304220		8	7.573187815	-3.250629719	-1.074987206
H	-0.08628438	2.16975151	2.34582141		8	4.561869875	-3.522985216	-0.700381917
C	0.79478336	-1.27850416	-0.70229433		8	5.680168186	-1.743627568	2.285203176
O	1.540462604	-1.38837262	-1.66943654		8	3.032800403	-2.327221114	3.053126461
H	3.71009959	-1.09191865	2.74186651		6	4.786765703	-4.592074466	-1.594914505
H	1.83652198	-2.40126596	1.57550442		6	4.845553946	-4.054684868	-3.041109465
H	3.31771309	-0.83621922	0.23793134		6	3.523171804	-3.342738237	-3.341777188
O	-0.41558058	-1.85394342	-0.67835806		6	2.367567021	-4.343595526	-3.181899379
H	-0.40123075	-2.63995133	-1.36904244		6	2.411442398	-4.970299412	-1.765108746
7a_gamma-CD_P:								
6	1.499441558	0.126653865	-1.452793604		8	1.443373111	-6.131990363	-1.550572563
6	1.121684960	-1.295969873	-0.955048563		8	5.942259639	-3.169458845	-3.218848953
1	2.026169113	-1.782622592	-0.534381257		8	3.607786368	-2.781486994	-4.642968183
6	0.212988218	0.815733900	-2.021224370		8	1.133965666	-3.650588562	-3.395504570
1	0.475734289	1.821260141	-2.412800696		8	3.726380545	-5.522589663	-1.517466346
6	0.027818451	-1.195191866	0.138313185		8	1.527556427	-7.119309514	-2.569986024
1	-0.235338405	-2.220714016	0.472233851		6	0.365208186	-4.017535170	-4.518735294
6	-0.8555290820	0.926217240	-0.912999472		6	-0.426312558	-2.783300225	-5.000704423
1	-1.754922883	1.427594930	-1.325776523		6	-1.480061864	-2.396679496	-3.953587031
6	-1.230411818	-0.492033134	-0.425280514		6	-2.400039629	-3.570924494	-3.628301030
1	-2.006899690	-0.420385990	0.365614896		6	-1.520691199	-4.774193848	-3.224013173
6	0.566947074	-0.376344081	1.334968485		6	-2.301023898	-6.070132484	-2.997773410
1	-0.213952336	-0.304755723	2.121869384		8	0.351641706	-1.658882499	-5.347128060
1	1.443053727	-0.885328947	1.786424387		8	-2.229782559	-1.269211391	-4.421300623
6	-0.285970227	1.754428960	0.261276245		8	-3.224632675	-3.207440950	-2.520809498
1	0.005224477	2.762259498	-0.104934430		8	-0.541568453	-5.068542290	-4.235298106
1	-1.050379781	1.913098926	1.043916489		8	-1.494991569	-7.095715919	-2.461792063
6	2.035825677	0.939562154	-0.243432504		6	-4.634119308	-3.338963288	-2.645293085
1	2.949032819	0.451176687	0.152276072		6	-5.267821737	-2.127412024	-3.368826078
6					6	-5.008337800	-0.857884021	-2.545034460
6					6	-5.525920881	-0.998856258	-1.110487167
1					6	-4.981424073	-2.315557619	-0.496226377

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6	-5.666031776	-2.712486424	0.825567315	1	1.016433965	-4.391859936	-5.332338842
8	-4.858453033	-1.937513223	-4.711869342	1	-0.953549748	-3.090628639	-5.925896668
8	-5.631036703	0.255761048	-3.200146326	1	-0.958335987	-2.114654100	-3.018244198
8	-5.025312256	0.094573743	-0.334648470	1	-3.011170479	-3.825858402	-4.518007797
8	-5.185956202	-3.445304155	-1.363188513	1	-1.013305644	-4.491895609	-2.279195585
8	-5.807374580	-1.655847927	1.756648705	1	-2.773176964	-6.362766656	-3.969195796
6	-5.939833472	0.982895817	0.308929450	1	-3.106878476	-5.872263745	-2.264263881
6	-6.491919910	2.058561994	-0.650545189	1	0.908304993	-1.381169411	-4.576309482
6	-5.301753339	2.817617682	-1.254816801	1	-1.596911043	-0.734693844	-4.954072017
6	-4.448864529	3.443188213	-0.152269997	1	-0.686127300	-7.177811694	-3.010596655
6	-4.099577297	2.396566178	0.942198049	1	-4.890664300	-4.281167920	-3.175225708
6	-3.572031602	3.060421540	2.227823740	1	-6.360499434	-2.313493393	-3.402685151
8	-7.363419424	1.596825444	-1.664691309	1	-3.914001186	-0.685540617	-2.497758849
8	-5.795909003	3.830398880	-2.154104539	1	-6.635018609	-1.011991104	-1.112071561
8	-3.185202181	3.925432076	-0.645029220	1	-3.893608250	-2.160488888	-0.333746318
8	-5.243247524	1.624802203	1.344944926	1	-5.104233655	-3.577164330	1.250737908
8	-2.332842913	3.715612561	2.052034286	1	-6.689016411	-3.067239576	0.586291228
6	-3.186947450	5.109255907	-1.442813618	1	-3.901234419	-1.663061597	-4.713192883
6	-2.759193265	4.787554632	-2.898794023	1	-5.569520366	0.072102400	-4.164175747
6	-1.287271543	4.381391588	-2.908660305	1	-5.000122926	-1.104690353	1.744562598
6	-0.416741588	5.486530398	-2.317098996	1	-6.755200038	0.406982062	0.786377474
6	-0.912347362	5.838891674	-0.890912820	1	-7.088429969	2.753943689	-0.026778840
6	-0.334763883	7.148137625	-0.311368153	1	-4.672837932	2.103380302	-1.818741162
8	-3.478097057	3.743019847	-3.516508817	1	-5.021271786	4.282030326	0.303012116
8	-0.841105769	4.122736914	-4.237343879	1	-3.326504979	1.725046303	0.520224538
8	0.932728137	5.003168352	-2.305208129	1	-3.432936277	2.269776378	2.992097444
8	-2.334829630	6.080178581	-0.893247693	1	-4.365315024	3.752660276	2.603866179
8	1.049824267	7.124302281	-0.070721333	1	-6.831442959	1.050651323	-2.305344228
1	1.466813547	6.388558142	-3.763990966	1	-6.625611282	3.450257905	-2.525752066
1	3.468358111	5.184878659	-4.480086198	1	-2.348906681	4.144361472	1.170833022
1	2.837732932	3.123453662	-2.308335921	1	-4.195430553	5.563964196	-1.432153194
1	5.144716985	5.137269572	-2.477098790	1	-2.863796076	5.740156777	-3.470463591
1	2.724284521	5.111434921	-0.581954917	1	-1.178102991	3.475278368	-2.278136162
1	4.740339078	6.030290205	0.478055917	1	-0.494106715	6.388636291	-2.961725003
1	3.573075478	7.340971206	0.111501689	1	-0.658604013	4.991992150	-0.219738985
1	1.007523636	3.824241844	-4.379668867	1	-0.837872824	7.319827310	0.660658957
1	5.351294490	2.964311262	-3.313898945	1	-0.640073030	7.978899100	-0.993622917
1	4.916682427	7.687447983	-1.823693345	1	-4.436994406	3.839142428	-3.275215638
1	6.615934805	4.948739815	-0.765873163	1	-1.502894132	3.524941172	-4.642240744
1	8.181855308	2.986995244	-0.950555848	1	1.528431798	7.100870328	-0.928625822
1	5.579577110	1.381085028	-1.254462332	8	3.620471260	0.736683772	-2.370455953
1	7.691968284	1.271828188	0.971167249	1	4.002812972	1.279662091	-3.146605813
1	4.819981735	2.352872907	1.054216597				
1	5.653309091	1.492452936	3.213323877				
1	5.519283750	3.288203463	3.243930039				
1	7.470239556	2.257519845	-3.084303674	6	0.393959815	-0.761708279	-0.611442726
1	7.972728333	0.015581534	-1.002223704	6	1.819892503	-1.239745579	-1.016083968
1	7.844774745	3.240187756	2.763505371	1	1.746243175	-1.920625060	-1.888145298
1	7.228593930	-0.448470172	2.521944578	6	0.501287941	0.155027232	0.632481083
1	7.951121359	-2.607843513	1.481645300	1	-0.504128390	0.504698552	0.932889843
1	6.290349523	-1.616977429	-0.905568596	6	2.710641559	-0.018285513	-1.342090496
1	5.909601872	-4.150395077	0.777800522	1	3.724875639	-0.373256755	-1.621701801
1	4.221834424	-1.572073649	0.799873553	6	1.395224004	1.371137893	0.306992693
1	3.067548457	-3.674555476	1.517065870	1	1.455584030	2.020760112	1.203909431
1	4.347931319	-3.942243137	2.757448372	6	2.807347796	0.898804012	-0.102105607
1	9.051552465	-1.717511962	-0.377116807	1	3.440945126	1.777240177	-0.338033881
1	7.202545688	-3.231176074	-1.993162476	6	2.098378428	0.784107701	-2.514538800
1	3.679716246	-1.745015383	3.501624712	1	2.751663882	1.647699454	-2.760102132
1	5.710533096	-5.143497099	-1.332309057	1	2.035906890	0.147256185	-3.423381590
1	4.952611409	-4.930915813	-3.718881580	6	0.769627326	2.167351666	-0.857346324
1	3.394192612	-2.543587932	-2.585838179	1	-0.241288548	2.507556862	-0.563599107
1	2.476705500	-5.162271752	-3.919456934	1	1.373026288	3.071384103	-1.072541714
1	2.194931993	-4.177558565	-1.019991195	6	-0.203331373	0.047680955	-1.810131337
1	0.401593884	-5.777896370	-1.547831891	1	-0.267971475	-0.618338800	-2.695852404
1	1.655120012	-6.562922119	-0.544891342	1	-1.236377715	0.366014255	-1.561842245
1	5.702386259	-2.583701134	-3.970409242	6	0.685097886	1.272272734	-2.115061403
1	3.153976511	-1.909405327	-4.611613061	1	0.235977937	1.845382633	-2.954562976
1	2.440846481	-7.466442900	-2.563894077	6	-0.519117616	-1.968073431	-0.409649645

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6	0.393959815	-0.761708279	-0.611442726
6	1.819892503	-1.239745579	-1.016083968
1	1.746243175	-1.920625060	-1.888145298
6	0.501287941	0.155027232	0.632481083
1	-0.504128390	0.504698552	0.932889843
6	2.710641559	-0.018285513	-1.342090496
1	3.724875639	-0.373256755	-1.621701801
6	1.395224004	1.371137893	0.306992693
1	1.455584030	2.020760112	1.203909431
6	2.807347796	0.898804012	-0.102105607
1	3.440945126	1.777240177	-0.338033881
6	2.098378428	0.784107701	-2.514538800
1	2.751663882	1.647699454	-2.760102132
1	2.035906890	0.147256185	-3.423381590
6	0.769627326	2.167351666	-0.857346324
1	-0.241288548	2.507556862	-0.563599107
1	1.373026288	3.071384103	-1.072541714
6	-0.203331373	0.047680955	-1.810131337
1	-0.267971475	-0.618338800	-2.695852404
1	-1.236377715	0.366014255	-1.561842245
6	0.685097886	1.272272734	-2.115061403
1	0.235977937	1.845382633	-2.954562976
6	-0.519117616	-1.968073431	-0.409649645

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8	-0.643435608	-2.844273102	-1.262781257	8	-4.556180246	-3.741074512	-2.133158741
1	3.294706940	0.357608454	0.733120531	8	-3.272371723	-3.648852358	0.729095244
1	0.914313049	-0.412637903	1.491230166	6	-5.059537990	0.586379373	-0.545868849
1	2.266759613	-1.818417533	-0.178964724	6	-5.611421960	1.726247996	-1.429872667
6	2.534804892	6.500790784	-1.885567607	6	-4.456960480	2.662099215	-1.820921552
6	3.540536734	5.749559849	-2.788707957	6	-3.754135813	3.187406003	-0.564448146
6	4.121142778	4.543462069	-2.017736737	6	-3.332420524	1.993242921	0.332635564
6	4.654296445	5.016106894	-0.656232410	6	-2.794609807	2.424960395	1.707684754
6	3.628791773	5.820639705	0.154594254	8	-6.329980617	1.305476977	-2.573920192
6	4.213533040	6.453231888	1.420207314	8	-4.989083813	3.744745144	-2.605553059
8	2.955122184	5.429012853	-4.023931097	8	-2.557543786	3.913422213	-0.865572263
8	5.146072276	3.939092601	-2.776914607	8	-4.452109835	1.127227430	0.591216931
8	5.029213858	3.838474130	0.064326300	8	-1.545520656	3.078387870	1.622890281
8	3.137438187	6.923802598	-0.661508741	6	-2.681502869	5.230603304	-1.417298532
8	5.364661079	7.243618187	1.148335914	6	-2.062686614	5.261678815	-2.836274001
6	6.186413480	3.857570126	0.868531020	6	-0.557993670	5.026292842	-2.720198003
6	7.169709340	2.792185529	0.346466003	6	0.096489370	6.051022370	-1.793779305
6	6.598107310	1.378954852	0.521200198	6	-0.631473524	6.093683248	-0.425355885
6	6.151049671	1.186704180	1.970848108	6	-0.282104841	7.310849781	0.459711633
6	5.199863922	2.315237525	2.414695277	8	-2.569280372	4.279375681	-3.716342032
6	4.820445914	2.227859608	3.892849431	8	0.076846676	5.099430551	-3.993768036
8	7.452849707	3.067555315	-1.020746247	8	1.452358843	5.638464208	-1.620613072
8	7.590044402	0.447535746	0.117048028	8	-2.061670646	6.178226447	-0.593485408
8	5.500787597	-0.081562052	2.056388870	8	0.985668542	7.251099653	1.060503079
8	5.860305064	3.583407971	2.222916002	1	2.191703715	7.426885154	-2.389410559
8	5.955775365	2.179958960	4.745287351	1	4.382149677	6.440039965	-3.001703297
6	5.761408059	-0.894684558	3.181942438	1	3.289168852	3.830154580	-1.824189423
6	6.670602741	-2.070018804	2.767773249	1	5.542778177	5.652672056	-0.839066399
6	5.950826505	-2.977428957	1.770934263	1	2.779072538	5.165025548	0.429083716
6	4.583215351	-3.402952703	2.321011166	1	4.530873027	5.648444661	2.107864380
6	3.7711181517	-2.178176066	2.769919566	1	3.410718564	7.040533289	1.920121770
6	2.468221508	-2.519254188	3.490996372	1	2.043930021	5.083740060	-3.871554497
8	7.875263525	-1.557659263	2.198573817	1	5.753798337	3.480535739	-2.151173495
8	6.798758676	-4.079634686	1.514146139	1	5.101033429	7.893171693	0.466666498
8	3.892000880	-4.077586003	1.268174362	1	6.649931321	4.862147769	0.871086168
8	4.549945760	-1.398118640	3.701785472	1	8.097615666	2.859856197	0.957492769
8	1.728998273	-1.355803559	3.806766041	1	5.702025444	1.288387409	-0.129838671
6	3.599867008	-5.442964918	1.386256651	1	7.046927608	1.206036808	2.622179861
6	4.042537604	-6.154744725	0.085713591	1	4.278694636	2.275696792	1.803136550
6	3.179412378	-5.675767939	-1.079914661	1	4.249747846	1.294379563	4.060313213
6	1.703667891	-5.900859287	-0.724194962	1	4.156886272	3.090851216	4.134606762
6	1.369074557	-5.128369049	0.563793691	1	7.951197333	2.294442129	-1.357339559
6	-0.080123886	-5.250279961	1.014068734	1	7.600634757	-0.304778816	0.757637271
8	5.426691490	-5.914611090	-0.145478234	1	6.507280402	2.954085086	4.513425392
8	3.575983921	-6.385869434	-2.244783231	1	6.220851828	-0.304307706	3.998616252
8	0.910883779	-5.462750665	-1.816598322	1	6.901890025	-2.661953865	3.681469712
8	2.213751563	-5.653136822	1.614135239	1	5.765436304	-2.381698594	0.847792516
8	-0.568003894	-6.593987708	1.021741343	1	4.740179414	-4.082546119	3.185664221
6	0.402034864	-6.460337723	-2.662780742	1	3.535099893	-1.561392026	1.880286053
6	0.369096681	-5.896728059	-4.093736693	1	1.839064415	-3.144466672	2.830038790
6	-0.619024846	-4.726642711	-4.158118408	1	2.714957793	-3.118200160	4.402337805
6	-2.009579433	-5.117368851	-3.609483132	1	8.325958782	-2.332754514	1.800539629
6	-1.844820075	-5.775890767	-2.212217695	1	6.365878171	-4.654374197	0.833905952
6	-3.093382594	-6.377796343	-1.550869347	1	2.351019485	-0.744670856	4.251086194
8	1.679690775	-5.509434269	-4.478973423	1	4.117346757	-5.890261513	2.258443312
8	-0.678112688	-4.180293428	-5.481472580	1	3.865161571	-7.245007219	0.223289177
8	-2.701561311	-3.874116299	-3.565067042	1	3.339505409	-4.582800000	-1.211535992
8	-0.896802764	-6.859950151	-2.291154753	1	1.522748630	-6.975279823	-0.520524804
8	-3.072904392	-6.227876672	-0.130830682	1	1.583048600	-4.050812730	0.414737181
6	-4.099471049	-3.793059652	-3.468164945	1	-0.709840378	-4.697587403	0.301502982
6	-4.474668974	-2.500409445	-4.228739367	1	-0.187848398	-4.773791848	2.013019238
6	-4.047274243	-1.253886444	-3.427476745	1	5.586489451	-6.113936719	-1.091538653
6	-4.567882551	-1.325428832	-1.986828547	1	3.107547706	-5.985327650	-3.013619125
6	-4.006295291	-2.634362675	-1.383362538	1	-0.078833789	-7.103505736	1.695402693
6	-4.277988893	-2.853828202	0.105960023	1	1.025028031	-7.375381867	-2.626134477
8	-3.913739074	-2.467714080	-5.531789404	1	-0.005338621	-6.716735133	-4.753746747
8	-4.529999456	-0.077266795	-4.079470953	1	-0.240186801	-3.910551320	-3.516043718
8	-4.103720405	-0.195829360	-1.261454859	1	-2.519880802	-5.819696563	-4.312462150

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

1	-1.453941437	-4.970908754	-1.565796649	H	-1.66833862	2.34479558	-1.80623711
1	-3.152021593	-7.451412546	-1.835516700	C	0.51906187	1.39634308	0.72031151
1	-4.010231703	-5.869310242	-1.882572644	H	0.44896817	1.27914107	1.81826898
1	1.584440542	-4.817552918	-5.165704684	H	1.25446983	2.19920749	0.52558784
1	-1.041452376	-4.870387213	-6.073954218	C	-0.84989559	1.80059446	0.15294825
1	-2.231685819	-6.597601396	0.244148476	H	-1.16818298	2.74458340	0.63075360
1	-4.586582612	-4.679513624	-3.926694719	C	2.40112903	-0.25271360	0.65484833
1	-5.574687745	-2.470450451	-4.351251695	O	2.80193640	-1.32996430	1.07264231
1	-2.937159352	-1.220407913	-3.384465848	C	-4.84436250	-3.61660783	-3.37435583
1	-5.677335039	-1.364936724	-1.997347030	C	-4.32843193	-3.22714571	-4.77320425
1	-2.908616108	-2.625073910	-1.512227602	O	-3.32538577	-4.10595036	-5.24694217
1	-5.287109502	-3.302023890	0.242626673	C	-3.84215939	-1.76669483	-4.77790061
1	-4.247646817	-1.872534818	0.614840213	O	-3.52629118	-1.34788991	-6.09864861
1	-2.969810800	-2.729390859	-5.424120768	C	-4.91185990	-0.83792516	-4.19999428
1	-4.380684898	-0.203002828	-5.040629270	O	-4.36638039	0.48024945	-4.20091598
1	-3.266548043	-4.589062172	0.374685560	C	-5.28893315	-1.32816993	-2.77966547
1	-5.889421904	-0.055642945	-0.182224445	O	-5.78630169	-2.68197616	-2.89852012
1	-6.330587981	2.296048176	-0.808203041	C	-6.36792278	-0.50682284	-2.04472690
1	-3.718997660	2.093995534	-2.422976600	O	-6.06526857	-0.30793182	-0.66649592
1	-4.462721459	3.835781586	-0.002385976	C	-5.17707595	1.55646269	-4.63378599
1	-2.539021413	1.432101181	-0.197551339	C	-4.32191929	2.47790413	-5.53421098
1	-2.655458966	1.510072332	2.316173586	O	-3.72001885	1.74602614	-6.57181726
1	-3.571212081	3.054111805	2.209244983	C	-3.32667034	3.30775837	-4.69215705
1	-5.709750236	0.819981844	-3.181101332	O	-2.81496771	4.34627394	-5.50989087
1	-5.716612311	3.340748234	-3.132206058	C	-3.99243590	3.89360328	-3.42821493
1	-1.613174899	3.715815627	0.882695767	O	-2.92245214	4.49838261	-2.67183280
1	-3.749034692	5.517858448	-1.451830544	C	-4.73934737	2.79895119	-2.64162832
1	-2.236131093	6.289771793	-3.235073009	O	-5.72854901	2.25391270	-3.53820955
1	-0.418701460	4.023597964	-2.272814268	C	-5.47982761	3.23335081	-1.36523990
1	0.053232781	7.051350424	-2.276405699	O	-5.39514386	2.25373508	-0.33453964
1	-0.352393915	5.172041555	0.125780717	C	-3.08396386	5.80574747	-2.16767018
1	-1.032399915	7.328997317	1.274950011	C	-1.69051186	6.48713492	-2.17390942
1	-0.432115727	8.237614773	-0.148273846	O	-1.00478740	6.30842313	-3.41386334
1	-3.542453398	4.186527855	-3.553410140	C	-0.79428384	6.02923168	-1.00757830
1	-0.415495630	4.492122298	-4.582703721	O	0.32718242	6.88802541	-0.86615682
1	1.688256297	7.337233029	0.375044490	C	-1.55447547	5.97558066	0.31983686
8	-1.198894000	-1.977401524	0.739165174	O	-0.66933589	5.40534652	1.27307338
1	-1.884898177	-2.732936231	0.738734197	C	-2.82517824	5.12820302	0.10119351
				O	-3.63816098	5.83074867	-0.86838736
				C	-3.66687466	4.80008433	1.35061921
				O	-3.80771795	3.38765984	1.47442931
				C	-0.57210601	5.96872546	2.57351230
				C	0.93147002	6.02129465	2.93111051
				O	1.63755679	6.78321242	1.98246255
				C	1.46596286	4.58798286	3.11739229
				O	2.75953820	4.64270769	3.68986591
				C	0.52246891	3.75388672	4.00806930
				O	0.96709333	2.39204789	3.90435754
				C	-0.95299102	3.84257326	3.58498589
				O	-1.32576981	5.23156679	3.50869958
				C	-1.92966689	3.14253227	4.54439885
				O	-2.99453307	2.49160074	3.85619031
				C	1.43504707	1.72733115	5.05319494
				C	2.60474914	0.80413141	4.58665092
				O	3.45020034	1.49828653	3.66837508
				C	2.09856541	-0.51900132	3.97827972
				O	3.14660274	-1.46496200	3.84471334
				C	0.92278614	-1.11665710	4.76434522
				O	0.50602437	-2.24886073	4.02141574
				C	-0.16284973	-0.02672178	4.86552311
				O	0.39782460	1.01469834	5.69680614
				C	-1.55813140	-0.43824359	5.38893174
				O	-2.57574660	-0.09959402	4.45080934
				C	0.10375923	-3.42557299	4.69343419
				C	0.85374476	-4.60316030	4.03965186
				O	2.25576044	-4.41665871	4.04807829
				C	0.32878767	-4.82363958	2.61113385
				O	0.88366564	-5.99938959	2.03515283

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C	-1.19907306	-4.93320816	2.59192128	H	0.64237482	-5.51802305	4.62903291
O	-1.56300269	-5.04759639	1.21786425	H	2.43604769	-3.46345059	3.85573867
C	-1.79511051	-3.66794897	3.26113271	H	0.60640471	-3.92823079	2.01245254
O	-1.28972779	-3.59889635	4.61259576	H	1.84607707	-5.95289303	2.21519009
C	-3.32461232	-3.56206393	3.35488868	H	-1.51467523	-5.83937623	3.15291508
O	-3.76918245	-2.21231057	3.24078641	H	-1.44484255	-2.78758072	2.68428369
C	-2.54327444	-5.97667598	0.81470732	H	-3.63211233	-3.95756057	4.34492307
C	-2.11138440	-6.50210205	-0.57251105	H	-3.79216541	-4.18971286	2.57612919
O	-0.79277011	-7.01549762	-0.56868024	H	-4.13671789	-2.07084205	2.31738558
C	-2.27906396	-5.40385821	-1.64410557	H	-2.61919337	-6.81090708	1.54150183
O	-2.09031551	-5.92921037	-2.95155675	H	2.78902641	-7.33709026	-0.84332443
C	-3.66728776	-4.75958427	-1.55875297	H	-0.26012751	-6.47426026	0.06004079
O	-3.71766439	-3.71640564	-2.52696018	H	-1.52462059	-4.61485535	-1.43361803
C	-3.86114552	-4.23799825	-0.11933438	H	-1.25638923	-6.44255303	-2.91973195
O	-3.82775151	-5.39076789	0.75287385	H	-4.44125322	-5.52522632	-1.77701036
C	-5.12221654	-3.41001714	0.18064374	H	-3.00304040	-3.58181141	0.11753816
O	-4.73779766	-2.14027965	0.70451608	H	-5.73763806	-3.97249270	0.91700690
H	-5.37968535	-4.58632389	-3.41965729	H	-5.72415149	-3.27222542	-0.73742936
H	-5.18122178	-3.29520223	-5.47877981	H	-5.25710355	-1.41068516	0.23745042
H	-2.79184617	-4.40650911	-4.47469843	O	3.21066490	0.84224121	0.69311782
H	-2.94842387	-1.70055031	-4.12271343	H	4.06185961	0.56080107	1.10114323
H	-2.96431914	-2.05526184	-6.47817843				
H	-5.81423424	-0.87901936	-4.84638214				
H	-4.37426626	-1.32348815	-2.15408191				
H	-7.32352250	-1.06552172	-2.12867562				
H	-6.49463568	0.47430851	-2.53725153				
H	-5.79941276	0.64980556	-0.51371979				
H	-6.04083172	1.17721106	-5.21551066				
H	-5.01168354	3.20869764	-6.00414244				
H	-3.44478291	0.87142234	-6.21389535				
H	-2.51670032	2.62047917	-4.34690695				
H	-2.36356077	4.98896837	-4.92617076				
H	-4.71852921	4.67405711	-3.73883765				
H	-4.01299871	2.01033598	-2.36015204				
H	-6.54581946	3.38822853	-1.63421961				
H	-5.07881377	4.19800029	-1.01044538				
H	-4.80317815	2.58963332	0.40577330				
H	-3.78969820	6.37942447	-2.80227399				
H	-1.85116416	7.57603296	-2.06711388				
H	-0.84462106	5.34464623	-3.49498021				
H	-0.46436781	4.98497258	-1.22070458				
H	0.72868730	6.98165564	-1.75371293				
H	-1.84692346	7.00401577	0.62054892				
H	-2.52339265	4.15612596	-0.32960492				
H	-4.66155773	5.28246163	1.23268857				
H	-3.18921746	5.20840494	2.26040817				
H	-3.53786519	3.05721353	2.38788168				
H	-0.99157158	6.99465765	2.58248248				
H	1.02913942	6.54221546	3.90442970				
H	1.31686446	6.52967338	1.08798145				
H	1.47975017	4.10417123	2.11311703				
H	3.10209232	3.72563588	3.75592816				
H	0.62563997	4.11316386	5.05363437				
H	-1.05403285	3.37048568	2.58939182				
H	-1.37138233	2.41195632	5.15890885				
H	-2.34336881	3.91649449	5.22633344				
H	-2.92423132	1.50261904	4.01152930				
H	1.80519118	2.45637610	5.80126686				
H	3.23132626	0.55878772	5.46354322				
H	2.88132931	1.72706260	2.90221482				
H	1.67095696	-0.28365394	2.98410259				
H	3.37269134	-1.50897590	2.88818051				
H	1.24813519	-1.41037028	5.78511120				
H	-0.34258762	0.37382800	3.84798809				
H	-1.73857846	0.10860499	6.33821410				
H	-1.59426097	-1.52335089	5.60007006				
H	-2.98317030	-0.91076033	4.01694951				
H	0.34608434	-3.36413716	5.77366852				

8a_beta-CD_S:

C	1.03702381	0.04450080	-0.01937627
C	-0.07822938	-0.98208013	0.34728156
H	-0.07833181	-1.12143536	1.44634227
C	1.05084072	0.20618091	-1.57834498
H	1.84668665	0.92502551	-1.85234491
C	1.31665241	-1.15662461	-2.25599473
H	2.30755692	-1.55207153	-1.94680998
H	1.35072445	-1.01898258	-3.35697740
C	0.17325033	-2.33964493	-0.34683240
H	-0.62722757	-3.04474375	-0.05275908
H	1.13010757	-2.77314794	0.00340694
C	0.19760688	-2.15418399	-1.87983630
H	0.38950946	-3.13166699	-2.37391359
C	-1.15831786	-1.58946213	-2.35168713
H	-1.13505106	-1.43895795	-3.45158740
H	-1.97942033	-2.29693141	-2.13519104
C	-1.45226031	-0.40904510	-0.10787869
H	-2.24541071	-1.13164391	0.17439123
C	-0.32475715	0.77341613	-2.02756391
H	-0.30494293	0.89811373	-3.13146703
C	-1.43323756	-0.24538118	-1.65536962
H	-2.41562345	0.14883393	-1.99048647
C	-1.74091719	0.95031163	0.56034168
H	-2.72863422	1.32981153	0.23121428
H	-1.79047502	0.83570879	1.66471706
C	-0.59729067	2.13112766	-1.35869431
H	0.20697666	2.84785100	-1.63319650
H	-1.55627631	2.54945308	-1.72520000
C	0.73165683	1.42459757	0.64966106
H	0.72719670	1.32235507	1.75185148
H	1.53405831	2.14206086	0.38797688
C	-0.63377406	1.95367155	0.17314221
H	-0.81591214	2.93353778	0.65239048
C	2.39583474	-0.40193745	0.51084405
O	2.59294727	-1.27605889	1.34412935
C	-5.03580813	-3.64742130	-3.36672895
C	-4.61965698	-3.27656740	-4.80309358
O	-3.65811280	-4.16831525	-5.33603994
C	-4.12305789	-1.82141714	-4.84944039
O	-3.88098345	-1.41372569	-6.18851032
C	-5.14955117	-0.87642134	-4.22153420
O	-4.57722285	0.42976501	-4.24942128
C	-5.47225278	-1.34773966	-2.78007830
O	-5.94756491	-2.71422170	-2.84071184

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C	-6.55724307	-0.53198937	-2.04909790	H	-5.56181059	-4.62335396	-3.35686633
O	-6.30495364	-0.38449969	-0.65246604	H	-5.51850457	-3.34711418	-5.44753051
C	-5.38418288	1.52717212	-4.63420480	H	-3.04642522	-4.42558109	-4.60788279
C	-4.53955364	2.45531389	-5.53847339	H	-3.19346151	-1.75866629	-4.24430518
O	-3.96911898	1.73304125	-6.60126506	H	-3.35564327	-2.13210963	-6.59835424
C	-3.51691119	3.26790489	-4.71029228	H	-6.07909205	-0.90161842	-4.82917106
O	-3.03251439	4.32218196	-5.52414891	H	-4.53918834	-1.30465493	-2.18334791
C	-4.14356440	3.82761068	-3.41493970	H	-7.51955970	-1.06890138	-2.17984757
O	-3.05891376	4.42280506	-2.67486123	H	-6.64890431	0.46619864	-2.51257391
C	-4.86169503	2.71415509	-2.63201205	H	-5.93947719	0.53574509	-0.47539438
O	-5.89159316	2.20805401	-3.50764707	H	-6.26992152	1.17303864	-5.19853229
C	-5.53404007	3.10195832	-1.30510602	H	-5.23353337	3.19921101	-5.98062195
O	-5.33009995	2.10119655	-0.31056456	H	-3.70822217	0.84668294	-6.26360099
C	-3.21671872	5.73069202	-2.16634508	H	-2.69619388	2.57462644	-4.40448895
C	-1.83131004	6.42444655	-2.21010440	H	-2.55642113	4.95171963	-4.94542840
O	-1.17430754	6.24294047	-3.46600029	H	-4.88332026	4.60859902	-3.68810323
C	-0.90786365	5.97695415	-1.06436759	H	-4.12913703	1.91326625	-2.40990379
O	0.21931871	6.83402962	-0.95954984	H	-6.62072590	3.22652041	-1.50092815
C	-1.63175393	5.93645443	0.28430750	H	-5.14165512	4.07228086	-0.95555620
O	-0.71985513	5.37282691	1.21401720	H	-4.84959552	2.50853691	0.47341329
C	-2.90851594	5.08387931	0.11789408	H	-3.94132063	6.29692344	-2.78603234
O	-3.74415932	5.75256213	-0.85828686	H	-1.99788130	7.51278650	-2.10682124
C	-3.73320484	4.82333204	1.39507095	H	-1.00146159	5.28093218	-3.54143020
O	-3.97292138	3.43000088	1.56145048	H	-0.58680551	4.93094896	-1.27661457
C	-0.54364295	5.96838611	2.49299926	H	0.59975308	6.91588407	-1.85749386
C	0.97471600	5.94779286	2.79004349	H	-1.91501190	6.96778979	0.58450850
O	1.68180543	6.63914248	1.78871536	H	-2.61548120	4.09289130	-0.27617593
C	1.43249217	4.49344238	3.01148585	H	-4.69427628	5.37324062	1.29696347
O	2.75807740	4.47474301	3.49016440	H	-3.19830505	5.21598160	2.28016694
C	0.49330053	3.78665402	4.01195777	H	-3.64593671	3.11032426	2.46168966
O	0.91312349	2.41739975	4.04315211	H	-0.90668222	7.01569296	2.48164410
C	-0.98691482	3.90114916	3.60760444	H	1.14068786	6.49574161	3.73937938
O	-1.30449719	5.30280999	3.47382641	H	1.30007537	6.38938655	0.91799900
C	-1.99189231	3.28167525	4.59342678	H	1.33890338	3.95743691	2.03775667
O	-3.06605178	2.61877438	3.92852379	H	2.99402393	3.53517595	3.66246915
C	1.21310194	1.81628024	5.27346107	H	0.63595124	4.25461329	5.00985704
C	2.43866339	0.89840579	5.08828805	H	-1.11973048	3.39295500	2.63347579
O	3.49809431	1.63459720	4.50034419	H	-1.46664612	2.56653180	5.25397983
C	2.06166943	-0.31486029	4.23052758	H	-2.39779440	4.10194194	5.22290263
O	3.20741846	-1.14702128	4.08023148	H	-2.98753824	1.62979709	4.08822132
C	0.85210573	-1.03616247	4.85399331	H	1.42259599	2.58159521	6.04687788
O	0.59158511	-2.18364867	4.05556761	H	2.73001592	0.53261575	6.09941771
C	-0.30483371	-0.00154127	4.88903140	H	4.16446895	0.96647176	4.23547416
O	0.11999686	1.06352531	5.76991525	H	1.74937111	0.06007018	3.23820647
C	-1.70506195	-0.46543221	5.34210577	H	3.22882390	-1.40183819	3.13045046
O	-2.72922100	0.01483198	4.47349987	H	1.09582788	-1.34339919	5.89390326
C	0.12126484	-3.36272547	4.68719703	H	-0.42937212	0.39680107	3.86159495
C	0.89200762	-4.56547307	4.09560929	H	-1.88100194	-0.05946618	6.35929421
O	2.28113245	-4.35057149	4.18939343	H	-1.75145262	-1.56762152	5.39251661
C	0.40602047	-4.88012642	2.66515340	H	-3.05318185	-0.71878934	3.87120078
O	0.89694066	-6.15862046	2.29813694	H	0.30321589	-3.31125405	5.77946568
C	-1.13433074	-4.84268049	2.55339478	H	0.65429263	-5.45176919	4.71732173
O	-1.41811611	-4.95675927	1.14314581	H	2.43845265	-3.40491331	3.97436540
C	-1.70157978	-3.54506623	3.15990837	H	0.79972723	-4.07954183	1.99638905
O	-1.26997198	-3.50555897	4.53419353	H	0.48919622	-6.39753636	1.44124835
C	-3.22912397	-3.37727226	3.16904033	H	-1.55484710	-5.71732831	3.09250608
O	-3.61264198	-2.02654157	2.93616288	H	-1.27569254	-2.68631978	2.60378269
C	-2.35241310	-5.90668003	0.68826603	H	-3.59459875	-3.69895235	4.16697918
C	-1.90434324	-6.34267201	-0.73399535	H	-3.68042854	-4.04731491	2.41786225
O	-0.50910944	-6.63891944	-0.79046704	H	-4.06699078	-1.95825178	2.04314057
C	-2.25957588	-5.30045393	-1.81212236	H	-2.37708171	-6.78376415	1.36638493
O	-2.11554304	-5.84028606	-3.11831524	H	-2.43025354	-7.28385978	-0.98175303
C	-3.68221947	-4.76011169	-1.64521822	H	-0.05013080	-5.80187375	-0.56571375
O	-3.84575919	-3.72348661	-2.60280678	H	-1.57314976	-4.43458642	-1.67613772
C	-3.82251931	-4.25543458	-0.19544126	H	-1.23279929	-6.26212745	-3.15449870
O	-3.67383606	-5.40694190	0.66606902	H	-4.41497227	-5.57603792	-1.82212142
C	-5.11817231	-3.49960475	0.15416273	H	-2.99615517	-3.54692271	0.00226492
O	-4.78125297	-2.16867431	0.53027559	H	-5.62048271	-4.03851918	0.98781783

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H	-5.80803403	-3.48143953	-0.71062762	O	-6.72383106	3.60894560	-1.02129272
H	-5.41598377	-1.49718283	0.11166672	O	-4.55928842	5.13606757	0.07519800
O	3.41786769	0.31839078	-0.00807570	O	-3.25138408	4.03252014	2.31302850
H	4.24551491	-0.00572401	0.41345992	O	-6.48875907	2.26336674	2.40574592
				O	-5.22439900	0.98722677	4.60643335
8a_gamma-CD_P:				C	-2.84820582	4.96125429	3.31379529
C	5.29676986	4.20145489	-2.22607424	C	-2.61686112	6.35135224	2.68283045
C	5.06284794	3.83681946	-3.70985361	C	-1.44617411	6.28190681	1.68968793
C	4.46422128	2.42068994	-3.78468975	C	-0.19825953	5.69158294	2.35408602
C	5.30582305	1.44100088	-2.94384024	C	-0.56894714	4.33880022	3.00962452
C	5.60654033	1.91970506	-1.51600737	C	0.56013540	3.70976523	3.83817797
C	6.66967160	1.07499641	-0.80789511	O	-3.75896192	6.91421931	2.06077146
O	4.29437211	4.83481678	-4.33203793	O	-1.18675720	7.61050011	1.20103584
O	4.41254037	1.99253438	-5.12608573	O	0.84250089	5.42268019	1.40323333
O	4.56768542	0.21371776	-2.88461751	O	-1.66918905	4.51522234	3.91901906
O	6.15237786	3.26820849	-1.57215424	O	1.68520903	3.34183487	3.03907957
O	7.89786124	1.05777896	-1.51908935	C	1.63478981	6.52660894	0.94593542
C	5.17590293	-0.98017087	-3.28714061	C	1.45549966	6.71920001	-0.58258858
C	4.19233956	-1.74224782	-4.19966937	C	2.10712755	5.55812372	-1.33236924
C	2.95715218	-2.20206587	-3.40199495	C	3.56750531	5.38951554	-0.91966279
C	3.44884324	-3.03925383	-2.21841802	C	3.64989034	5.22304088	0.61438676
C	4.40609347	-2.19331019	-1.35436791	C	5.07632007	5.18153724	1.20563574
C	4.98416495	-2.96825672	-0.16985029	O	0.11199960	6.77763224	-1.01193637
O	3.81970862	-0.91630597	-5.29204726	O	2.03659551	5.75866291	-2.73992939
O	2.05227047	-2.88638786	-4.25632533	O	4.04595697	4.22285498	-1.57601583
O	2.33875187	-3.50626589	-1.45743207	O	2.98425246	6.32421369	1.27111315
O	5.52450738	-1.79635347	-2.17252314	O	5.70511047	3.92989620	1.09181346
O	5.63754358	-4.16257281	-0.57542340	H	5.80510492	5.18377504	-2.15276436
C	2.36688672	-4.87825568	-1.09106159	H	6.04551047	3.82300524	-4.22235266
C	1.72209377	-5.77912418	-2.17006351	H	3.45122021	2.46769940	-3.32416091
C	0.22379407	-5.51204768	-2.30717120	H	6.27200709	1.28584085	-3.46500074
C	-0.46214105	-5.57255284	-0.93524571	H	4.67202178	1.92759293	-0.92155644
C	0.27273901	-4.65752487	0.05569598	H	6.31650841	0.02883846	-0.75668072
C	-0.24531261	-4.71552775	1.48988974	H	6.79020502	1.46445850	0.23033811
O	2.36756825	-5.59901770	-3.43747067	H	3.44652174	4.93363841	-3.83832292
O	-0.27899346	-6.47267727	-3.21623209	H	4.08395201	1.06301100	-5.12932639
O	-1.80782327	-5.11739585	-1.09646369	H	8.15063093	1.99313473	-1.65277273
O	1.66509107	-5.04130458	0.11481849	H	6.13129835	-0.78667336	-3.81383487
O	0.40499028	-3.76353574	2.30824606	H	4.71856604	-2.65305712	-4.56813279
C	-2.88606197	-6.00722191	-0.97344408	H	2.43879656	-1.29912331	-3.02229338
C	-3.78472027	-5.87470880	-2.22188968	H	4.03022855	-3.89563172	-2.60994970
C	-4.36217236	-4.46323361	-2.27702632	H	3.86946497	-1.29631336	-0.97835480
C	-5.09419969	-4.16194845	-0.96546884	H	4.15741637	-3.26183885	0.50456974
C	-4.17371097	-4.38221327	0.24922825	H	5.67089905	-2.29277899	0.39183160
C	-4.88424716	-4.22744176	1.59613318	H	3.02071714	-1.33156767	-5.68033606
O	-3.04265668	-6.17523595	-3.39946988	H	2.15004577	-3.85638641	-4.08386745
O	-5.22048700	-4.39056654	-3.40471082	H	6.28698174	-3.90175439	-1.25947466
O	-5.53236756	-2.80482022	-1.01628755	H	3.40781559	-5.20092479	-0.89274464
O	-3.65181120	-5.72987672	0.18912539	H	1.85801254	-6.83057176	-1.83309294
O	-6.12482496	-4.91985927	1.66439125	H	0.09989345	-4.47618463	-2.69673659
C	-6.89507988	-2.55354765	-1.21006703	H	-0.44469031	-6.61902349	-0.56306283
C	-7.04065860	-1.39023830	-2.21705905	H	0.20219341	-3.61485291	-0.30184282
C	-6.46273945	-0.10400833	-1.61702437	H	-1.32571957	-4.47737294	1.49334234
C	-7.02586548	0.18178503	-0.21490483	H	-0.12030292	-5.75903499	1.87284233
C	-6.90919157	-1.08258021	0.66111423	H	1.82887484	-6.12371664	-4.06912240
C	-7.54948200	-1.00304945	2.04522589	H	-1.23998984	-6.28628645	-3.37147276
O	-6.39175327	-1.73020995	-3.43610211	H	1.36467314	-3.89482577	2.16923232
O	-6.61992521	1.00013942	-2.52174070	H	-2.53292722	-7.05182415	-0.86101105
O	-6.24308586	1.24272735	0.31354604	H	-4.62393933	-6.59660441	-2.10967993
O	-7.53741701	-2.19279563	-0.00438617	H	-3.51684460	-3.74756066	-2.37238922
O	-7.24245418	-2.14421302	2.81783733	H	-5.96130001	-4.84269551	-0.85945971
C	-6.85639973	2.28684708	1.05151274	H	-3.33631425	-3.65710026	0.20963008
C	-6.43025612	3.60570547	0.36607047	H	-5.11932668	-3.16521956	1.77971534
C	-4.93512898	3.86751008	0.61320087	H	-4.17972823	-4.55966599	2.39269301
C	-4.63933983	3.82496231	2.11279241	H	-3.54259860	-5.78137585	-4.14532091
C	-5.07207130	2.44599336	2.65487408	H	-5.50234214	-3.45101854	-3.51380441
C	-4.86377534	2.27816527	4.16026699	H	-5.93371495	-5.87233736	1.56181393
				H	-7.42350341	-3.45106272	-1.58665319

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H	-8.13416552	-1.24747981	-2.38693506	H	-1.61397413	-0.91790770	1.01140111
H	-5.37389088	-0.23160260	-1.51906085	H	-0.00540890	-1.44798022	0.45877246
H	-8.09640400	0.48052407	-0.29865548	C	-1.56862904	-1.57413726	-1.07641645
H	-5.82823726	-1.28428202	0.79285593	H	-1.81709320	-2.62479104	-0.83330571
H	-8.65133745	-0.85633959	1.91871083	C	-0.03345423	1.17605065	1.13730126
H	-7.13723837	-0.12455436	2.57561305	O	-0.76785383	1.35898126	2.09716394
H	-6.16466868	-0.89394788	-3.89227251	O	1.27566528	1.46935606	1.15469398
H	-7.57749739	1.18630477	-2.61750891	H	1.46600775	2.00498163	1.99426775
H	-7.43251005	-2.94127310	2.27886193				
H	-7.96026928	2.18085019	1.03172307				
H	-7.00888107	4.43806903	0.81287973				
H	-4.34602901	3.06479677	0.12088299	8a_gamma-CD_S:			
H	-5.23614559	4.61612780	2.61423206	C	0.37420680	0.47871729	0.06473709
H	-4.50021694	1.65309877	2.13229100	C	0.36792942	0.66701235	1.59782072
H	-5.42833707	3.08400224	4.69207680	C	1.82532334	0.70308047	2.09487553
H	-3.78541753	2.40678335	4.37307169	C	2.58302766	-0.52255336	1.54481331
H	-6.35184131	2.77822494	-1.40343431	C	2.45611706	-0.72302450	0.02592483
H	-5.01206102	5.22141351	-0.79054005	C	2.98042603	-2.08250480	-0.44604001
H	-6.17338712	0.86515011	4.41090015	O	-0.40927039	1.78305090	1.93803579
H	-3.60893162	5.02335202	4.11923035	O	1.84982332	0.69593633	3.50442212
H	-2.33820237	7.04324334	3.50255471	O	3.96694210	-0.35235637	1.88030563
H	-1.73330077	5.62009880	0.84624973	O	1.05308184	-0.70269027	-0.34102113
H	0.16868116	6.39538724	3.13414551	O	2.29941017	-3.15896876	0.17647353
H	-0.85803816	3.62650994	2.21799783	C	4.60370854	-1.29759054	2.69251318
H	0.16697458	2.78488128	4.29562422	C	5.43982087	-0.54379021	3.74889144
H	0.86686346	4.41446503	4.64436472	C	6.55909246	0.25556396	3.05072911
H	-4.03646262	6.32651935	1.30945082	C	7.39436100	-0.71448166	2.22326648
H	-2.07543958	8.02405850	1.11093569	C	6.49307296	-1.45707465	1.21517689
H	1.85950253	4.09703594	2.43398914	C	7.24763239	-2.50835694	0.40117692
H	1.33060707	7.44489388	1.48402941	O	4.59540053	0.30981268	4.50688786
H	2.00505630	7.65562684	-0.84294932	O	7.29846219	1.00586463	3.99685326
H	1.56686902	4.63397382	-1.04541317	O	8.41382558	0.01437578	1.54738705
H	4.14521042	6.28481149	-1.23642633	O	5.45808092	-2.15193175	1.93422730
H	3.16006486	4.25872975	0.86650406	O	7.92367022	-3.44707254	1.22463827
H	4.96630511	5.39981141	2.28694366	C	9.71357365	-0.54627143	1.55469524
H	5.67663531	6.01347572	0.76023762	C	10.55722289	0.01499356	2.72270958
H	-0.41419194	7.28174834	-0.33896118	C	10.84198041	1.50602440	2.54372013
H	1.10155826	5.95981261	-2.94618732	C	11.41411913	1.77821949	1.14653516
H	5.97654266	3.77840603	0.15628613	C	10.49665183	1.16851473	0.07885994
C	-0.55601373	0.57673871	-0.17661411	C	10.99920174	1.29645711	-1.35524612
C	-1.84681870	1.36915677	-0.58370422	O	9.88662905	-0.21691098	3.96759343
H	-2.53926081	1.36205588	0.28212575	O	11.72369117	1.89051331	3.58067910
C	0.42692623	0.62799599	-1.38979597	O	11.47177651	3.19660257	0.98423528
H	1.35814733	0.08958184	-1.11796645	O	10.34587177	-0.24501726	0.33504917
C	0.76681303	2.07916117	-1.78847360	O	10.00832169	0.89654695	-2.28376735
H	1.29655611	2.57892047	-0.95864021	C	12.69548046	3.83803809	0.75197269
H	1.45661345	2.06502264	-2.65655961	C	12.81980086	5.01079121	1.74801073
C	-1.48861890	2.82708716	-0.95385703	C	11.74750110	6.05445621	1.44283228
H	-2.41448048	3.39065092	-1.19913830	C	11.86570088	6.47379562	-0.02694434
H	-1.02501794	3.34250529	-0.08832552	C	11.74894746	5.25331681	-0.95502589
C	-0.52098995	2.84587382	-2.15705854	C	11.95444872	5.58241375	-2.43466243
H	-0.26859487	3.89498355	-2.41447837	O	12.71142683	4.52136012	3.08062102
C	-1.19310057	2.15551491	-3.36343589	O	11.93967892	7.14203443	2.33538516
H	-0.51217172	2.17685943	-4.24043081	O	10.84381626	7.43109202	-0.30349906
H	-2.12153159	2.69716611	-3.64927712	O	12.78633238	4.31637403	-0.58159247
C	-2.50969087	0.65341355	-1.79065481	O	13.12154275	6.35927873	-2.67584981
H	-3.44040534	1.20264370	-2.05881402	C	11.25586093	8.77110401	-0.36853483
C	-0.24419861	-0.08535141	-2.60344638	C	10.18889446	9.65796672	0.30814139
H	0.46491164	-0.06201725	-3.45789826	C	8.89393580	9.67417885	-0.51226379
C	-1.52978748	0.69647830	-2.99539428	C	9.17291020	10.00233580	-1.98852798
H	-2.00344984	0.19034840	-3.86441254	C	10.27411305	9.06153850	-2.52019815
C	-2.85495726	-0.80516518	-1.43397663	C	10.72540897	9.30218981	-3.95978461
H	-3.37472101	-1.29465794	-2.28369809	O	9.96951202	9.20101145	1.63449899
H	-3.54800242	-0.83180030	-0.56662035	O	7.92973414	10.55390790	0.08702771
C	-0.58990583	-1.54543784	-2.26573042	O	7.94724885	9.81821111	-2.67872261
H	0.33374506	-2.10353649	-2.01999133	O	11.44803429	9.19840147	-1.69905518
H	-1.04314183	-2.04254257	-3.14936276	O	11.53960155	8.25385150	-4.43588922
C	-0.92009341	-0.90258182	0.14708953	C	7.59610302	10.69172697	-3.74279280
			C	6.22276577	11.29638233	-3.37573624	

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C	5.13205824	10.21933064	-3.46142765	H	12.51942854	5.30249852	3.64100009
C	5.17728665	9.46594920	-4.79124663	H	11.17622051	7.75745530	2.23553816
C	6.60235830	8.93061612	-5.03325302	H	13.89167307	5.83312658	-2.38516831
C	6.79665005	8.25120913	-6.38870427	H	12.22821140	8.91269564	0.14133252
O	6.23457002	11.89102983	-2.08593758	H	10.60463009	10.69454375	0.31573653
O	3.84128912	10.80079174	-3.30219741	H	8.43119329	8.67251230	-0.46629843
O	4.26052786	8.38811439	-4.68356904	H	9.51978630	11.05854186	-2.06928035
O	7.55110809	10.02266642	-4.97515596	H	9.88143122	8.02723941	-2.45114918
O	8.05456132	7.61510621	-6.48693134	H	11.23455442	10.29758259	-4.00413052
C	3.37668546	8.07320878	-5.75219970	H	9.83055045	9.33928865	-4.60770337
C	1.94267741	8.35208047	-5.26120289	H	9.10029259	9.54409299	1.92627140
C	1.58982665	7.38379628	-4.11702387	H	8.29508453	11.46334826	0.06474031
C	1.80366369	5.93779204	-4.58417358	H	12.25433870	8.08171446	-3.78591481
C	3.27394725	5.80334803	-5.05376239	H	8.35515207	11.49164486	-3.85529244
C	3.64151542	4.38802875	-5.52561753	H	5.98422183	12.10093441	-4.09760682
O	1.72926171	9.69416956	-4.87011937	H	5.32530061	9.47691316	-2.65637225
O	0.23374871	7.62462313	-3.71801965	H	4.88614729	10.16043249	-5.60824492
O	1.58534292	4.97640807	-3.55473843	H	6.83975635	8.19475464	-4.24142976
O	3.52147031	6.72830027	-6.13087664	H	6.63653303	9.01125913	-7.19287518
O	3.83310030	3.51234233	-4.42960727	H	6.02752491	7.46253768	-6.49832510
C	0.22295897	4.69263251	-3.20248498	H	6.56910732	11.20515559	-1.46037055
C	0.01897352	4.99653965	-1.69035084	H	3.88150949	11.37604115	-2.51089063
C	0.69491135	3.92701468	-0.82372344	H	8.74413013	8.29843530	-6.37935087
C	0.27127807	2.52892122	-1.28980672	H	3.61150272	8.68062876	-6.64964654
C	0.55523583	2.34603086	-2.79324630	H	1.24736484	8.15791765	-6.10187944
C	0.10102916	0.98909504	-3.37718847	H	2.27038973	7.57240361	-3.25942086
O	0.51727254	6.26403997	-1.31845131	H	1.13553028	5.72848698	-5.44967637
O	0.34893337	4.09106698	0.54602383	H	3.93976848	6.05261764	-4.20613350
O	1.01725723	1.58474226	-0.53508298	H	4.60161771	4.44837793	-6.07452959
O	-0.12141967	3.37497104	-3.53612188	H	2.86350179	4.01616302	-6.23519105
O	1.01459102	-0.05789837	-3.14886194	H	2.43360231	9.96073642	-4.22660716
H	-0.66606528	0.37233780	-0.30334606	H	0.12897421	8.60244356	-3.75732876
H	-0.12245285	-0.21855446	2.05235089	H	3.03207282	3.59756998	-3.87225370
H	2.30369132	1.61983045	1.67732868	H	-0.44757923	5.33133436	-3.80541925
H	2.17714978	-1.42642203	2.04076076	H	-1.07907778	4.92192812	-1.50459091
H	2.98743583	0.09435418	-0.50244957	H	1.79179296	4.00646927	-0.95663084
H	4.04573140	-2.17421583	-0.16550189	H	-0.81747879	2.40704843	-1.10441773
H	2.89632554	-2.12070433	-1.55851345	H	1.65191330	2.40356348	-2.95403764
H	-0.03566762	2.58604019	1.48866523	H	0.02977396	1.13075237	-4.47424112
H	2.79358816	0.70021896	3.78766434	H	-0.92784373	0.75647195	-3.00656239
H	1.34576240	-3.00283541	0.02357586	H	0.24966345	6.90417625	-2.02155488
H	3.87120716	-1.97180060	3.17822134	H	1.10219750	4.53061330	0.99535524
H	5.91298993	-1.30589917	4.41055066	H	0.99085421	-0.32173092	-2.20166786
H	6.05740919	0.96989716	2.36575938	C	5.20006154	4.87284779	0.95857686
H	7.84222712	-1.46833418	2.90069812	C	4.81490985	4.33064247	-0.45101042
H	6.04553273	-0.71304406	0.52210938	H	4.09593750	3.49714526	-0.32170219
H	8.01629701	-2.00235858	-0.21350831	C	6.19497371	6.06402592	0.76158617
H	6.52383543	-3.00773077	-0.28465986	H	6.46958444	6.47021504	1.75500270
H	5.18744397	0.95883576	4.94204114	C	5.54397358	7.17243631	-0.10018920
H	8.19830880	0.60024445	4.07137609	H	4.64045690	7.56752859	0.40886832
H	7.25259279	-3.80724867	1.83940558	H	6.25128080	8.02235147	-0.20767474
H	9.66169924	-1.65107483	1.61386646	C	4.17570782	5.44248163	-1.30830661
H	11.52824610	-0.52642475	2.71759772	H	3.90195276	5.01408540	-2.28804035
H	9.87114039	2.04743824	2.61400040	H	3.23841138	5.81289489	-0.85083880
H	12.42917122	1.33238305	1.07494435	C	5.17166837	6.60777272	-1.48920423
H	9.50771686	1.65971354	0.14708789	H	4.70004379	7.39904610	-2.10620357
H	11.24359556	2.35531477	-1.56182021	C	6.45035643	6.09676672	-2.18886166
H	11.93990398	0.70093075	-1.45565635	H	7.17351277	6.93172739	-2.31590531
H	10.42026622	0.25804681	4.64013863	H	6.20312051	5.71164243	-3.19950671
H	11.94871947	2.84710745	3.46099474	C	6.09566792	3.79724166	-1.15192123
H	9.71236856	0.00711416	-2.00362616	H	5.80275227	3.40894830	-2.14839831
H	13.54642690	3.13803182	0.87507404	C	7.47501457	5.52107641	0.06360435
H	13.81696544	5.48128987	1.59609396	H	8.19543277	6.35901345	-0.05495601
H	10.75061886	5.58599798	1.59270452	C	7.08957953	4.97849001	-1.33948864
H	12.86339358	6.92057006	-0.20688299	H	8.00488532	4.60064366	-1.84373909
H	10.75300661	4.78063716	-0.83162939	C	6.74949760	2.67801467	-0.31708637
H	11.10626856	6.18037742	-2.80905746	H	7.63879182	2.28252901	-0.85036638
H	11.97259402	4.62482120	-3.00239795	H	6.03870113	1.83295699	-0.19361999

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C	8.12627677	4.40781146	0.90729130	C	3.18917398	-1.12067824	-2.63473641
H	8.41275216	4.80362106	1.90547889	O	1.95457758	-0.63606177	-2.13869051
H	9.05761456	4.05344522	0.42400593	C	6.55665145	0.20282176	-2.28739051
C	5.87771788	3.73672306	1.79293598	C	7.69311378	0.96669936	-1.56573750
H	5.14723014	2.91276300	1.92541453	O	8.62986033	0.07049035	-1.01874948
H	6.14155617	4.11904874	2.79984274	C	7.09308430	1.94935400	-0.53446434
C	7.14237137	3.23183996	1.06992047	O	8.10972347	2.83445899	-0.09240296
H	7.61149752	2.43616720	1.67745883	C	5.91378834	2.74455551	-1.13088065
C	3.94755657	5.25512916	1.73758624	O	5.28434978	3.45179574	-0.04367834
O	2.84447745	4.75931381	1.58153009	C	4.89552267	1.83151661	-1.82925722
O	4.17697476	6.16761055	2.71481990	O	5.60051887	1.08414558	-2.83826691
H	3.32395163	6.28732102	3.19132697	C	3.70756015	2.54178065	-2.49775407
				O	2.50115758	2.15106914	-1.84897920
9a_beta-CD_P				C	5.32234469	4.86258641	-0.04625058
C	0.46482257	5.99600921	1.97267974	C	5.29733994	5.30187064	1.43932902
C	-0.05735653	5.57895218	3.35688186	O	6.26988279	4.59478697	2.21215228
O	0.91317029	5.72175788	4.37972404	C	3.90255267	5.10480695	2.04780833
C	-0.54720033	4.12214318	3.28284553	O	3.79051448	5.69853613	3.33773198
O	-1.08734633	3.73120054	4.54270066	C	2.78535011	5.64770981	1.15662237
C	-1.57294726	3.91095537	2.16336697	O	1.57169749	5.15977246	1.71447185
O	-1.77332075	2.51437732	1.98288296	C	2.94979611	5.09526720	-0.27261565
C	-1.00080684	4.49248951	0.83918824	O	4.25904384	5.44064620	-0.77336122
O	-0.54988079	5.84755108	1.00086665	C	1.88231084	5.59601571	-1.26720521
C	-2.04469568	4.47895139	-0.26673955	O	1.21701560	4.50728077	-1.90718349
O	-1.42873568	4.87130912	-1.50103304	H	0.75764657	7.06524388	1.95433680
C	-3.10397898	1.97769536	2.00636095	H	-0.91222367	6.23163880	3.62399048
C	-3.61570045	1.78830247	3.46034012	H	1.79714340	5.48366660	4.00931067
O	-3.71536395	3.02061650	4.13463065	H	0.32414810	3.48683514	3.03928291
C	-2.72212672	0.74342118	4.14192900	H	-0.47993257	4.08618522	5.22587424
O	-3.17646699	0.48828814	5.45630783	H	-2.51985620	4.42152478	2.43011050
C	-2.71007760	-0.54596503	3.28663971	H	-0.14758487	3.85391219	0.53125320
O	-1.83721998	-1.48221986	3.91767316	H	-2.86482920	5.18354064	-0.00580097
C	-2.24450325	-0.26081356	1.84220282	H	-2.44917176	3.44747326	-0.33730928
O	-3.08319662	0.77821515	1.28865306	H	-2.06209994	4.75370251	-2.23274533
C	-2.37299729	-1.43487063	0.84695692	H	-3.79401097	2.65700752	1.46128465
O	-1.38678612	-2.43937014	1.03152597	H	-4.64444010	1.37738587	3.38739565
C	-2.42902601	-2.40510867	4.80799968	H	-2.82871452	3.24588780	4.50299860
C	-1.47317848	-2.62014428	6.00161913	H	-1.68580047	1.14210385	4.15721648
O	-1.23885276	-1.36876972	6.63752277	H	-2.45512133	0.01259090	5.93043467
C	-0.19411288	-3.26100532	5.47803997	H	-3.74152918	-0.95577676	3.23767007
O	0.67614679	-3.53635844	6.57036739	H	-1.19163728	0.07921277	1.86234643
C	-0.43746637	-4.51695237	4.61507444	H	-2.32644864	-1.00014290	-0.17397808
O	0.88048658	-4.71398424	4.05249384	H	-3.37048239	-1.90627382	0.97204742
C	-1.52623644	-4.22826209	3.55483624	H	-0.66977683	-2.43333305	0.34779528
O	-2.68088903	-3.64167841	4.18799613	H	-3.40619919	-2.03499075	5.16866511
C	-2.06409819	-5.40475159	2.72845541	H	-1.97157096	-3.32164591	6.70668291
O	-2.59310366	-4.98376636	1.47953981	H	-0.33388497	-1.33867854	7.01434188
C	1.24075308	-5.89392486	3.40558243	H	0.27116039	-2.52332675	4.79413143
C	2.78343573	-6.04345740	3.51416605	H	1.50123904	-3.88372635	6.17175588
O	3.28773152	-5.86417268	4.83655824	H	-0.70318581	-5.38406709	5.25905125
C	3.51138001	-5.01533431	2.63490156	H	-1.07837499	-3.48766202	2.86843765
O	4.90183940	-5.31856377	2.56368144	H	-2.87926216	-5.88446638	3.31186424
C	2.93442878	-5.01282184	1.21683192	H	-1.26457190	-6.15580962	2.57298852
O	3.59244700	-3.99673220	0.46956195	H	-2.17829229	-4.12123664	1.23606566
C	1.41195903	-4.79811353	1.29505541	H	0.72493635	-6.77171114	3.85425000
O	0.87902170	-5.91282201	2.03346011	H	3.04001432	-7.05184038	3.12109633
C	0.66667743	-4.71039817	-0.05252366	H	3.03390234	-6.63639121	5.37663597
O	0.61978529	-3.38787993	-0.57140098	H	3.35539382	-4.00783099	3.07667187
C	3.96510104	-4.28993836	-0.87382807	H	5.23193699	-5.38374864	3.48171513
C	5.50431756	-4.35124296	-0.96496268	H	3.12496932	-6.00961762	0.76439537
O	6.06605700	-5.29540980	-0.07455228	H	1.20154406	-3.85676273	1.83831076
C	6.09653381	-2.95338148	-0.74769613	H	1.09427515	-5.42282597	-0.79289819
O	7.50562462	-2.95780149	-0.92118819	H	-0.37955605	-5.01087242	0.14820491
C	5.47898620	-1.94591238	-1.71622309	H	1.48662260	-3.12560468	-0.95319091
O	5.97767861	-0.66339428	-1.33106116	H	3.53270574	-5.25968057	-1.18933231
C	3.93539708	-1.97711196	-1.59699602	H	5.77279863	-4.68566124	-1.98699043
O	3.42946244	-3.33110201	-1.74747223	H	5.71556343	-5.12928810	0.83539495
				H	5.82986457	-2.63025536	0.28479321

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H	7.82941562	-3.75479126	-0.45051071	O	0.60843746	6.44552427	3.35606167
H	5.79261320	-2.19220454	-2.75311316	C	-1.06706104	4.71388622	2.98200761
H	3.68028819	-1.62146165	-0.58466080	O	-1.38216679	4.72626998	4.36584130
H	3.00035461	-1.77646601	-3.51358927	C	-2.30953370	4.39224521	2.14622230
H	3.85445238	-0.30355812	-2.97158903	O	-2.76521926	3.08609539	2.46132211
H	2.03963489	0.33887607	-1.99187094	C	-1.92400618	4.45585566	0.64710990
H	6.97126502	-0.37346678	-3.13879380	O	-1.34635226	5.73966420	0.31024453
H	8.22167759	1.57591459	-2.32731962	C	-3.10764324	4.21519824	-0.29226336
H	8.14300512	-0.72859633	-0.71678192	O	-2.74111309	4.21200672	-1.65847207
H	6.69333793	1.33718408	0.30687988	C	-4.14141377	2.86979077	2.79687173
H	7.73438738	3.38969763	0.62123744	C	-4.25906932	2.61400097	4.32405916
H	6.31466151	3.46830148	-1.87008551	O	-3.91366766	3.76203383	5.05156988
H	4.48447105	1.13571110	-1.07403054	C	-3.44319151	1.35254782	4.65825675
H	3.69940341	2.25341913	-3.57265203	O	-3.57590661	1.00281178	6.01891213
H	3.83678757	3.64221290	-2.44569946	C	-3.91372510	0.18971251	3.76493367
H	1.87539710	2.92817553	-1.88656173	O	-2.94545981	-0.85640115	3.91936326
H	6.24802364	5.22553459	-0.53571769	C	-3.99903277	0.53881923	2.26932963
H	5.57239274	6.37171123	1.49474672	O	-4.64968228	1.80288698	2.03801422
H	6.04272879	3.64522232	2.11176182	C	-4.78043875	-0.50925239	1.47817543
H	3.73170045	4.01280753	2.11996820	O	-4.47571684	-0.49402193	0.08591928
H	4.55052579	5.37627592	3.86451566	C	-3.33505785	-2.13768789	4.32117287
H	2.80758347	6.75890738	1.15351226	C	-2.26748421	-2.66753512	5.29560657
H	2.85960180	3.99578213	-0.20852314	O	-2.12188613	-1.75533270	6.37285319
H	2.39897713	6.22351747	-2.02531467	C	-0.94778312	-2.88239845	4.54819387
H	1.13340848	6.22164956	-0.74343372	O	-0.03058057	-3.44928281	5.47156494
H	0.23433992	4.60460254	-1.79496969	C	-1.16903839	-3.77537247	3.31463190
C	2.43054623	1.80632154	3.07234495	O	0.09064733	-3.89913830	2.63230863
C	1.27718389	0.89653087	3.57130037	C	-2.27695839	-3.16602094	2.42534675
H	0.33491936	1.21475299	3.08401769	O	-3.46240759	-3.03756598	3.23019183
C	3.73900769	1.37440523	3.78352334	C	-2.63180136	-4.00685165	1.19356289
H	4.57058119	2.03335090	3.44412604	O	-3.66313577	-3.45250316	0.40382248
C	3.58010992	1.50695737	5.31119359	C	0.64576626	-5.18147455	2.43980986
H	3.35580611	2.55869222	5.58363782	C	2.09152050	-5.21605769	3.00102446
H	4.52141054	1.23206408	5.82875050	O	2.19770235	-4.77676919	4.36177979
C	1.10724561	0.99928307	5.09709106	C	3.01855503	-4.32715662	2.17291107
H	0.28412966	0.33821118	5.42656203	O	4.36650531	-4.45863105	2.61485510
H	0.83698207	2.03698207	5.37808786	C	2.93752611	-4.74517522	0.70314973
C	2.43438013	0.58973029	5.80305224	O	3.73542743	-3.84450469	-0.05538748
C	2.77071096	-0.87927369	5.41319679	C	1.47039566	-4.73053196	0.22306007
H	3.72764927	-1.17458416	5.89399211	O	0.67064807	-5.57022271	1.08667144
H	1.98985397	-1.55931879	5.79797997	C	1.26925383	-5.25069011	-1.21952552
C	1.58761051	-0.56909028	3.16758116	O	1.46159523	-4.27799847	-2.21679830
H	0.74652416	-1.20641611	3.50161913	C	4.63186497	-4.36209490	-1.03145089
C	4.05905500	-0.08935547	3.37581508	C	6.08197318	-4.10160784	-0.57585058
H	5.00483602	-0.40506482	3.86673455	O	6.39193166	-4.70179160	0.66424614
C	2.90138839	-0.99342303	3.88229935	C	6.34078405	-2.58902170	-0.54998119
H	3.12694912	-2.04731676	3.61827035	O	7.68506141	-2.30494694	-0.19269031
C	1.74488750	-0.69448438	1.64068978	C	6.05402013	-1.97815655	-1.91855874
H	1.95992102	-1.74428744	1.35846739	O	6.15383665	-0.56451420	-1.74722756
H	0.79950943	-0.41951685	1.13259700	C	4.63894299	-2.35437263	-2.41987603
C	4.20081819	-0.20461680	1.84478504	O	4.38115448	-3.77950235	-2.28614822
H	5.03745767	0.43291785	1.49027508	C	4.42836548	-2.01407804	-3.90633198
H	4.44741762	-1.25170618	1.57414720	O	3.07524135	-1.78872219	-4.23554414
C	2.56805553	1.68142240	1.54437697	C	6.76187386	0.25904895	-2.72238759
H	1.63299718	2.01501256	1.05059791	C	7.63710924	1.27283088	-1.95318373
H	3.38524006	2.32321111	1.16652998	O	8.59611200	0.60840106	-1.16764706
C	2.88192959	0.22396449	1.16484478	C	6.72970350	2.22831419	-1.14615591
H	2.96473027	0.15567279	0.06785628	O	7.50713607	3.32314566	-0.69286700
C	2.27888869	0.71142048	7.31370242	C	5.52753786	2.73702298	-1.97912319
O	2.92179702	1.42712912	8.05034845	O	4.58193824	3.34750531	-1.08150929
H	2.21451376	2.85807114	3.35266773	C	4.81898283	1.62379488	-2.77129600
O	1.28649380	-0.10649734	7.79941217	O	5.80029262	0.91020495	-3.53094366
H	1.25473562	0.03922249	8.77126664	C	3.77876328	2.17548409	-3.73861486
9a_beta-CD_S:				O	3.08687637	1.09379436	-4.36368189
C	-0.19201303	6.06841285	1.05101484	C	4.63156345	4.75452036	-0.92289842
C	-0.50109163	6.08290513	2.56121964	C	4.57151281	5.04333912	0.59688952
				O	5.50777654	4.23889520	1.32629188
				C	3.16328780	4.83694352	1.16738771

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

O	3.07968367	5.36156180	2.49012638	H	4.86888979	6.09415382	0.76856711
C	2.09530379	5.50205875	0.29676744	H	5.25320600	3.31010451	1.13135024
O	0.83384311	5.11555533	0.82445043	H	2.94344973	3.74596145	1.16958788
C	2.26850097	5.03440462	-1.16307796	H	3.82646613	4.99232079	3.00292177
O	3.58985638	5.40755543	-1.60775593	H	2.22320465	6.60497253	0.34489778
C	1.24531109	5.61491901	-2.15904628	H	2.16219783	3.93496076	-1.19905851
O	0.03656818	4.88940083	-2.17318101	H	1.70951688	5.52947968	-3.16382267
H	0.12129611	7.07392288	0.70555009	H	1.08912159	6.70115072	-1.96173977
H	-1.28123892	6.84862245	2.74335933	H	0.59655475	5.26178099	-1.51993695
H	1.39652654	5.91368419	3.07907602	C	0.51074912	1.27752641	-1.23092352
H	-0.29995674	3.93554052	2.77053560	C	1.13285419	0.02174296	-1.89541909
H	-0.67182309	5.23790280	4.80875921	H	2.16855676	0.24776545	-2.21227013
H	-3.09120802	5.14881546	2.36830589	C	-0.95195448	0.93215831	-0.84088728
H	-1.15866645	3.67527404	0.46727793	H	-1.42718133	1.81452902	-0.36675729
H	-3.83684422	5.04116996	-0.17011235	C	-1.76874271	0.52396410	-2.07992882
H	-3.59901581	3.26603973	0.02267237	H	-1.80470263	1.34523828	-2.82448414
H	-2.09028540	3.50103611	-1.82005811	H	-2.81107330	0.29405897	-1.78343154
H	-4.74574282	3.75839007	2.52500929	C	0.32746292	-0.39310246	-3.14030657
H	-5.32690999	2.41003783	4.54408887	H	0.79269080	-1.28001887	-3.60929148
H	-2.95688793	3.95916688	4.91555245	H	0.31690572	0.43469377	-3.88116924
H	-2.38085969	1.56161909	4.39472882	C	-1.13805125	-0.72934430	-2.73807701
H	-3.02495019	0.20004636	6.16006089	C	-1.09618612	-1.89489898	-1.71917181
H	-4.90533170	-0.14202638	4.14033526	H	-2.12711964	-2.18866426	-1.44136662
H	-2.96129434	0.59699225	1.89297351	H	-0.61078496	-2.77506773	-2.17857801
H	-5.86647919	-0.33515884	1.65937012	C	1.16330076	-1.13061818	-0.85843503
H	-4.52859631	-1.52282687	1.83457106	H	1.61868688	-2.02221839	-1.32630962
H	-4.60903744	0.41727733	-0.23952146	C	-0.93085785	-0.21992326	0.19551303
H	-4.33048674	-2.12158493	4.80857267	H	-1.97642094	-0.46011567	0.46597302
H	-2.61567239	-3.65907574	5.66427303	C	-0.29952630	-1.46423503	-0.47214134
H	-1.29638466	-2.00280002	6.83714331	H	-0.30195023	-2.29239919	0.26553860
H	-0.59192443	-1.88977899	4.19325889	C	1.96747046	-0.71946556	0.39085673
H	0.82760767	-3.56266351	5.00190510	H	1.98753462	-1.55953145	1.11592166
H	-1.50988125	-4.77458249	3.65964025	H	3.02253231	-0.50592972	0.11012139
H	-1.94933391	-2.15991285	2.09189655	C	-0.13102976	0.19962892	1.44538501
H	-3.00205706	-4.99512461	1.53432291	H	-0.60523683	1.08732013	1.91628948
H	-1.69433728	-4.17645647	0.61586423	H	-0.14364892	-0.61845718	2.19707583
H	-3.43525038	-2.54145985	0.12959072	C	1.32543598	1.67662314	0.01609867
H	0.02906565	-5.94989006	2.95227451	H	2.37096273	1.90490431	-0.28356973
H	2.45638797	-6.26166823	2.91388110	H	0.90180388	2.59619982	0.46679987
H	1.85643897	-5.47856347	4.95029745	C	1.32507343	0.52431842	1.04214847
H	2.67851045	-3.27393483	2.26496188	H	1.90471278	0.82555469	1.94151832
H	4.37793632	-4.29533005	3.57877962	C	-1.89629253	-1.05605506	-4.02280811
H	3.33672599	-5.77963835	0.62214867	O	-2.32528915	-0.22698686	-4.80128202
H	1.09602521	-3.69379751	0.26973798	H	0.50293696	2.12268389	-1.95240120
H	1.90251293	-6.15784486	-1.37622024	O	-2.01147261	-2.39156320	-4.24962751
H	0.21150118	-5.57360625	-1.28598756	H	-2.47103990	-2.48404046	-5.11454478
H	2.41570338	-4.06987207	-2.33524276				
H	4.46565771	-5.44980484	-1.16774433				
H	6.76011848	-4.55954751	-1.32370166				
H	5.70179183	-4.45238812	1.32859103				
H	5.63180125	-2.13454861	0.18041769				
H	7.90188118	-2.91794354	0.54152714				
H	6.82523379	-2.33530964	-2.63484879				
H	3.90611095	-1.79640197	-1.80518909				
H	4.80215281	-2.88277665	-4.49056399				
H	5.04440192	-1.13009759	-4.16376060				
H	2.94202787	-0.81526086	-4.22224523				
H	7.38719073	-0.34157898	-3.41190771				
H	8.18722470	1.88437641	-2.69562043				
H	8.15258125	-0.15100881	-0.72612316				
H	6.31207524	1.63597924	-0.29859149				
H	7.05495240	3.73713944	0.07329017				
H	5.90874253	3.48954850	-2.70020012				
H	4.32017631	0.93460885	-2.05954931				
H	4.29483129	2.80247012	-4.50122932				
H	3.08422475	2.81849047	-3.15784832				
H	2.27194043	1.43051159	-4.77894411				
H	5.57266532	5.15657565	-1.34269330				

9a_gamma-CD_P

C	-0.17183488	0.05077177	0.02599014
C	-0.14455205	0.31909256	1.55071958
C	1.31748551	0.47428456	2.02595511
C	2.09990998	-0.77374645	1.58665359
C	2.01293100	-0.96324174	0.06413666
C	2.71397504	-2.22743519	-0.42965108
O	-0.91880877	1.47144058	1.89494761
O	1.39533958	0.71843104	3.41430898
O	3.46340876	-0.60994111	1.95553807
O	0.61341258	-1.08114119	-0.32344557
O	2.26837948	-3.39902539	0.24096794
C	4.09485295	-1.68389880	2.63040179
C	3.85594457	-1.61898195	4.15500559
C	4.42876233	-0.31958660	4.73799211
C	5.90466027	-0.20416967	4.35201513
C	6.07346761	-0.34909136	2.82453549
C	7.54200741	-0.39001596	2.40158237
O	2.46199593	-1.71696707	4.46733041
O	4.19119182	-0.29558304	6.14212070

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O	6.39756658	1.06834006	4.75882243	O	1.70734243	-0.08883172	-2.93098001
O	5.47933391	-1.59257730	2.38742591	H	-1.20266588	-0.19355287	-0.30368704
O	8.27598550	-1.39942072	3.07904253	H	-0.58163647	-0.56920880	2.05678244
C	7.56490982	1.11058456	5.55714511	H	1.75224918	1.35056984	1.51003502
C	7.26500472	0.89808599	7.05674640	H	1.66599404	-1.66863981	2.07320548
C	6.27880354	1.95539002	7.55047209	H	2.45748997	-0.08425394	-0.44130769
C	6.76386364	3.37252878	7.20786147	H	3.79648335	-2.12936974	-0.22436703
C	7.24731162	3.47723567	5.74897942	H	2.57805003	-2.29754311	-1.53332722
C	8.03223210	4.75705454	5.46332353	H	-1.45689784	1.77882306	1.11358106
O	6.73750276	-0.41147146	7.31113010	H	1.62759881	-0.13125015	3.86094468
O	6.12090848	1.75486102	8.94552771	H	1.29540998	-3.42438478	0.14592761
O	5.66985673	4.27950267	7.34481613	H	3.76133861	-2.65715255	2.21704554
O	8.13771208	2.38802283	5.41698901	H	4.39757891	-2.48253761	4.60348985
O	8.40993782	4.84564027	4.10370040	H	3.87056029	0.52506567	4.28859969
C	5.49435002	5.02157964	8.52313580	H	6.47508780	-1.02029464	4.83630294
C	4.09560736	4.72733702	9.11388944	H	5.57247113	0.50499905	2.32600844
C	3.02765640	5.14716612	8.10565717	H	8.01149164	0.57886613	2.65817152
C	3.23577678	6.62479975	7.75418842	H	7.58382100	-0.51851410	1.29460537
C	4.66414856	6.87440652	7.24509312	H	2.41494079	-1.54116083	5.43375438
C	4.96349475	8.35278270	6.98914836	H	5.04997116	-0.47868139	6.60177928
O	3.96801389	3.34932182	9.45026529	H	7.79845625	-2.23926527	2.92563022
O	1.75847306	4.88831501	8.68509540	H	8.31549075	0.37714341	5.19622699
O	2.29895551	6.99207599	6.74895678	H	8.23023138	1.01604776	7.59636359
O	5.59792378	6.41140937	8.24879036	H	5.32126834	1.79583932	7.01255843
O	4.62961628	9.18652245	8.09095695	H	7.58993627	3.64246952	7.90171525
C	1.10297080	7.59042721	7.19505631	H	6.36203923	3.43602681	5.08552063
C	-0.07390833	6.95046660	6.41640858	H	7.39099406	5.62948141	5.69255219
C	-0.07930481	7.41772818	4.95133712	H	8.91870134	4.78682305	6.14363437
C	0.08079233	8.93916385	4.83798265	H	6.47987964	-0.38456943	8.25980557
C	1.32031717	9.36670729	5.64513688	H	5.28995749	2.22419292	9.21645358
C	1.67829832	10.85098882	5.64263040	H	8.81520333	3.98418777	3.87691561
O	-0.03898895	5.53132717	6.53343567	H	6.28571705	4.79393397	9.26472285
O	-1.26834679	7.01632495	4.26838850	H	3.98321397	5.34914981	10.02930607
O	0.27885506	9.22116189	3.45688907	H	3.16823533	4.55039378	7.17796827
O	1.13961059	8.98841760	7.01877419	H	3.09268995	7.24819739	8.65948481
O	2.96376100	11.05749315	6.19494329	H	4.82268234	6.30726945	6.30586939
C	-0.33900415	10.35768059	2.87986578	H	4.36004368	8.71283696	6.13737266
C	-1.49612018	9.87082606	1.98618636	H	6.04013117	8.44416760	6.71427304
C	-0.92293612	9.05059261	0.82205628	H	3.00661888	3.15341809	9.45062877
C	0.18219135	9.79117246	0.06120502	H	1.07013127	4.98838946	7.97585906
C	1.22559054	10.32572891	1.07419938	H	5.12800658	8.85697452	8.86451476
C	2.28776471	11.26381613	0.47717865	H	0.96076047	7.42248575	8.27904644
O	-2.47079840	9.11578295	2.68268708	H	-1.01408908	7.29776988	6.88964985
O	-1.98383015	8.68746843	-0.06923522	H	0.79849780	6.97499910	4.44472651
O	0.81716238	8.84465914	-0.80150107	H	-0.83143181	9.44096621	5.22357043
O	0.59203814	11.08396799	2.11884487	H	2.18842008	8.82533840	5.21657461
O	2.93231757	10.75692114	-0.67802859	H	0.88127611	11.41440450	6.18845937
C	0.90102471	9.10010994	-2.20140926	H	1.71309939	11.21525657	4.59747735
C	-0.40984829	8.74004466	-2.93679693	H	0.42744219	5.14627784	5.74819488
C	-0.71823927	7.25381384	-2.70966141	H	-1.22075788	6.04428760	4.15660122
C	0.45469821	6.37636419	-3.13958127	H	3.01290354	10.58797298	7.05464294
C	1.77985108	6.89207601	-2.52086091	H	-0.70862490	11.05036771	3.66236349
C	3.01916430	6.22557269	-3.14314201	H	-2.01604794	10.75873658	1.57489090
O	-1.53746703	9.53258062	-2.60698151	H	-0.46870366	8.13058631	1.24459670
O	-1.90725220	6.90454303	-3.44894392	H	-0.25093835	10.63333341	-0.51526667
O	0.31109681	5.02357861	-2.67565345	H	1.72353058	9.44112560	1.51718679
O	1.93980876	8.30614938	-2.71201982	H	3.01350847	11.49715781	1.29026814
O	3.12725102	4.85786464	-2.80123543	H	1.79594342	12.21322295	0.18281898
C	-0.63278014	4.17632287	-3.32506046	H	-2.02095385	8.35443186	3.13391819
C	-1.77200939	3.79133949	-2.34504433	H	-2.75680101	8.47219867	0.49749890
C	-1.17342915	2.97909689	-1.19995871	H	3.06936277	9.79462497	-0.57967706
C	-0.42505070	1.75510894	-1.71707254	H	1.19282227	10.15263106	-2.37983740
C	0.57696397	2.12430345	-2.83647227	H	-0.22025035	8.90916304	-4.01573457
C	1.03180590	0.90345467	-3.66723765	H	-0.89629357	7.08863463	-1.62963098
O	-2.46017571	4.87834149	-1.76524145	H	0.52788592	6.39390810	-4.24979094
O	-2.20669184	2.52434886	-0.30921353	H	1.75014307	6.65870575	-1.43903621
O	0.31093074	1.19578226	-0.63203200	H	3.91854914	6.74038928	-2.75479900
O	-0.00348575	3.01533431	-3.80544477	H	2.98883412	6.38340460	-4.24921870

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H	-1.80959691	9.30972499	-1.67700503	C	5.87656889	-0.48186398	0.10274580
H	-2.46629489	7.71495206	-3.42243058	C	6.47037954	-0.81429518	-1.26466025
H	2.23360208	4.47166029	-2.90681343	O	4.68572448	-0.88457697	4.08298711
H	-1.04715452	4.68308252	-4.21713570	O	7.18754542	0.36227644	3.57431198
H	-2.46726535	3.13627285	-2.92193474	O	7.77079679	0.89915286	0.78978477
H	-0.45530953	3.62145877	-0.65058237	O	5.11233489	-1.63369690	0.52569523
H	-1.16803103	1.02581619	-2.11011666	O	7.40204827	-1.88712120	-1.20663578
H	1.45623448	2.58969221	-2.34487736	C	9.10613946	0.61131265	0.42014372
H	1.73278659	1.26954242	-4.44291735	C	10.04227472	0.51871681	1.64752382
H	0.12818462	0.50791003	-4.19298091	C	10.03459990	1.84347372	2.40801439
H	-2.51647982	5.61556520	-2.43005349	C	10.40807691	2.99995086	1.46876625
H	-2.76235948	3.30870373	-0.11470878	C	9.51768720	2.96685336	0.21109424
H	1.10046766	-0.47401449	-2.26479139	C	9.94846582	3.95733005	-0.87332167
C	5.38881574	5.63089629	2.51829523	O	9.66106021	-0.54534919	2.52799457
C	4.64547121	4.97320054	1.32602814	O	10.93217077	1.70907132	3.50008939
H	5.34940411	4.31576549	0.77371340	O	10.17991431	4.24073161	2.12809675
C	4.36713207	6.50531046	3.29006865	O	9.57638383	1.65977860	-0.40003996
H	4.87297356	6.96845188	4.16276086	O	9.15128393	3.81545511	-2.05664689
C	3.18647060	5.64567519	3.78711886	C	11.19872013	4.78324227	2.94108860
H	3.56000252	4.83442115	4.44768304	C	10.62861500	5.08145248	4.34769586
H	2.50869682	6.25834733	4.40434980	C	9.48462999	6.07713620	4.19947755
C	3.44474960	4.12801443	1.80295460	C	9.96970712	7.32739544	3.45794697
H	2.93945237	3.67306147	0.93067012	C	10.65478175	6.96847130	2.12494898
H	3.78698232	3.30092756	2.46061310	C	11.34595451	8.14919354	1.44159153
C	2.44064156	5.02336179	2.58416295	O	10.18683611	3.87742686	4.96895075
C	1.94718974	6.15911504	1.63029114	O	8.97052482	6.37518235	5.48879547
H	1.23170466	6.81433891	2.16937083	O	8.81221244	8.12976034	3.21552357
H	1.41501609	5.70727284	0.76959781	O	11.68508004	5.98523345	2.37942001
C	4.15315235	6.09454946	0.37058818	O	12.14929872	8.91990840	2.32716155
H	3.64815282	5.61973277	-0.49285695	C	8.70694109	9.38556567	3.81873267
C	3.86833269	7.63980776	2.34923072	C	7.24736875	9.56887605	4.28601116
H	3.14699620	8.27536843	2.90755193	C	6.32117070	9.58421990	3.06758071
C	3.14479551	6.98437581	1.14283564	C	6.78628571	10.53688533	1.95040260
H	2.77076619	7.77296110	0.45815779	C	8.29859595	10.37234267	1.68035728
C	5.33126344	6.95826324	-0.12426428	C	8.94224845	11.44150720	0.79033945
H	4.95267878	7.74923373	-0.80915529	O	6.90104074	8.52449239	5.18781659
H	6.03994577	6.33179172	-0.70524949	O	4.96176723	9.82115657	3.45466633
C	5.05080566	8.49650368	1.85351484	O	5.98554115	10.14111130	0.85024200
H	5.55519521	8.98048151	2.71621015	O	9.02546489	10.43419343	2.92388304
H	4.67488950	9.30784274	1.19183247	O	10.32286460	11.19747310	0.60913793
C	6.56731147	6.49124808	2.01905451	C	5.79583160	10.95875507	-0.28852249
H	7.29768275	5.84765100	1.48772974	C	4.28660099	10.87128804	-0.57793975
H	7.10312436	6.92680737	2.88586350	C	3.93562741	9.44543456	-1.02685720
C	6.05033685	7.60466587	1.08182395	C	4.83797421	8.94382609	-2.16229840
H	6.90095192	8.22161886	0.72559302	C	6.31592614	9.12525090	-1.73598681
H	5.77919938	4.84170610	3.19305354	C	7.35990360	8.78129201	-2.81212542
C	1.18379589	4.25936893	3.00419370	O	3.50654111	11.23174547	0.55701190
O	0.58762697	4.39688511	4.07303077	O	2.55985185	9.39667689	-1.42121508
O	0.74275100	3.48495554	2.02052187	O	4.52561155	7.56868371	-2.37757951
H	0.01675695	2.81531489	2.26278719	O	6.54660813	10.51349120	-1.38523356
9a_gamm-CD_S:							

C	-0.40624436	0.52424431	1.08668090
C	0.06578302	0.72369902	2.54321819
C	1.60360559	0.65214674	2.55645703
C	2.11642738	-0.58834476	1.80580201
C	1.47259598	-0.81816486	0.43072394
C	1.78212312	-2.19470824	-0.16145913
O	-0.45996718	1.92174599	3.06466865
O	2.07980713	0.65000344	3.88735798
O	3.52143231	-0.37094472	1.64933758
O	0.02492884	-0.73243638	0.56065942
O	1.48023631	-3.25880007	0.73195301
C	4.41368262	-1.44987200	1.74865763
C	5.40938885	-1.13800225	2.88554962
C	6.28384763	0.07207096	2.51453316
C	6.95765643	-0.20895388	1.16875698

C	1.80878225	6.68908470	-3.17025000
C	2.08514522	5.19676740	-3.36605019
C	3.57230430	4.95476384	-2.99541406
C	4.01075253	3.48781877	-3.14794549
O	2.41295075	8.86359126	-4.07039467
O	0.44672476	7.03848028	-3.46833463
O	1.31726583	4.34870490	-2.51376104
O	4.42657057	5.76707576	-3.80993592
O	3.51404493	2.67786874	-2.09247980
C	-0.10703702	4.31105439	-2.65349961
C	-0.71854902	4.78766757	-1.31453345
C	-0.23082365	3.82255070	-0.23368496
C	-0.59589130	2.37310883	-0.57382021
C	-0.22238007	1.98438123	-2.03187423
C	-0.93910432	0.71865267	-2.55985140

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

O	-0.32470969	6.09544381	-0.94230474	H	1.91062537	4.92091401	-4.42998239
O	-0.77082302	4.12265244	1.05134892	H	3.70431034	5.22384457	-1.92878779
O	0.14850989	1.57840496	0.34333389	H	5.11480753	3.46092962	-3.09481260
O	-0.55999601	3.02315738	-2.96449279	H	3.69556188	3.10856146	-4.14963147
O	-0.35382448	-0.49573091	-2.16178199	H	2.41236893	9.17197640	-3.12570604
H	-1.51350084	0.52141892	1.02788992	H	0.48684769	7.97732135	-3.76340080
H	-0.33321109	-0.10314616	3.16343018	H	2.57234446	2.92269976	-1.97870227
H	1.97157312	1.53901826	1.99662752	H	-0.42389442	4.95166994	-3.49447792
H	1.92911452	-1.47626726	2.44168781	H	-1.82694229	4.70865249	-1.40787558
H	1.82424747	-0.03483042	-0.26804505	H	0.87671648	3.89237466	-0.21034644
H	2.86567009	-2.25067158	-0.37423314	H	-1.68758648	2.23934312	-0.41256677
H	1.23413488	-2.28660591	-1.12615270	H	0.86926858	1.78778246	-2.06246802
H	-0.32236145	2.64083143	2.40335517	H	-0.87250835	0.76500255	-3.66453452
H	3.00886382	0.32071286	3.87009767	H	-2.02358211	0.78404782	-2.29275433
H	0.53730103	-3.16490133	0.97287573	H	-0.28472998	6.64602259	-1.76193333
H	3.87749605	-2.40113415	1.93106738	H	-0.53826665	5.05359256	1.24101241
H	6.07435999	-2.02367561	3.01283937	H	-0.42796434	-0.60973542	-1.18536282
H	5.62017646	0.95007864	2.40955232	C	4.53477288	6.15019158	3.46128980
H	7.57331544	-1.12401387	1.25706514	C	3.69178705	5.91960368	2.17775035
H	5.21550719	0.40330443	0.00260031	H	2.87163579	6.66949771	2.14375646
H	7.01746400	0.07275004	-1.63687910	C	5.69695065	5.11973298	3.47343100
H	5.63475496	-1.02863420	-1.97013138	H	6.33328639	5.30259095	4.36679786
H	5.33086870	-0.47389856	4.69756213	C	6.56846796	5.26346368	2.21104544
H	8.05313356	-0.06023275	3.34644521	H	7.03158665	6.26838281	2.16950685
H	6.93685924	-2.63450648	-0.77954086	H	7.38954381	4.51790686	2.23517807
H	9.15092718	-0.31341448	-0.18920318	C	4.57552678	6.09220362	0.92660820
H	11.06721762	0.32709937	1.25921054	H	3.96494826	5.99122059	0.00912504
H	8.99899820	2.02133638	2.76527347	H	5.02799152	7.10335397	0.91700185
H	11.47474169	2.90142423	1.16869260	C	5.71305242	5.03507938	0.93040751
H	8.47281612	3.17782751	0.50614891	C	5.10155272	3.61449402	0.99274190
H	9.80300745	4.99052070	-0.51248551	H	5.91927391	2.86678170	0.99886357
H	11.02298385	3.80381198	-1.11824585	H	4.49154391	3.41817801	0.08936294
H	10.24177086	-0.42335882	3.31278404	C	3.07571978	4.49472174	2.24386660
H	10.65911476	2.37100460	4.18570556	H	2.45994574	4.31952248	1.33661231
H	9.14033066	2.85552162	-2.26402708	C	5.08725340	3.69506549	3.54565146
H	12.06371486	4.09576131	3.00800662	H	5.91250512	2.95212745	3.57639439
H	11.44236484	5.54263577	4.94984130	C	4.24163983	3.46828253	2.26167818
H	8.71188590	5.59532104	3.57367255	H	3.82071613	2.44547124	2.29561928
H	10.69815328	7.87572582	4.08789392	C	2.19437003	4.35010271	3.50275123
H	9.89334851	6.54855625	1.43556276	H	1.72773363	3.34774669	3.54188386
H	10.60039391	8.84125038	1.01858926	H	1.36734068	5.09326102	3.46547579
H	11.94367654	7.73876865	0.59501800	C	4.19802188	3.53506148	4.79683210
H	9.52802777	4.12692332	5.64994571	H	4.80974283	3.66829062	5.71534916
H	8.18273738	6.95685159	5.36831689	H	3.76397903	2.51473566	4.81594815
H	12.84366801	8.32556842	2.67326573	C	3.66100144	5.99778049	4.72286809
H	9.40596714	9.48719638	4.67184941	H	2.85119980	6.75985714	4.71168661
H	7.19375849	10.56068181	4.79469360	H	4.27875656	6.18107337	5.63043863
H	6.32148260	8.56965749	2.63445140	C	3.05545496	4.57761840	4.76656400
H	6.56698249	11.59242321	2.23753668	H	2.42356794	4.46378345	5.67036263
H	8.43611195	9.37709339	1.21298480	H	4.95201222	7.17420312	3.42869141
H	8.75005000	12.44435711	1.24830044	C	6.63974045	5.23549670	-0.26955836
H	8.47873239	11.41163043	-0.21232053	O	7.31671820	6.24826440	-0.44832667
H	5.92653351	8.42668789	5.17141827	O	6.70448619	4.17972431	-1.08382933
H	4.92052555	10.70482007	3.87482960	H	7.53075314	4.23971275	-1.66189263
H	10.71739775	11.05224766	1.49488345				
H	6.10713408	12.00428851	-0.08647776				
H	4.02931418	11.58383142	-1.38498998				
H	4.08991283	8.76395208	-0.16595088				
H	4.65347778	9.54473473	-3.07575569				
H	6.50089383	8.48442480	-0.85242220				
H	8.35109338	9.10613837	-2.40938896				
H	7.16414161	9.38360133	-3.72379090				
H	3.85372755	10.68544040	1.30015174				
H	2.06244145	9.92142194	-0.75798763				
H	7.41639093	6.88684536	-2.36791318				
H	4.94099123	7.61334185	-4.41889440				
H	2.60732964	7.15189615	-5.13146029				
H	2.02526723	6.94995249	-2.11526041				

10a_beta-CD_P:

C	1.22154797	-5.79778896	1.87366551
C	2.64125602	-6.14153961	2.38853370
O	2.67835410	-6.18827944	3.79683779
C	3.67627649	-5.16088563	1.79739178
O	5.01420742	-5.59114596	2.01924431
C	3.48647038	-4.94597458	0.29142513
O	4.36948447	-3.88538192	-0.06360288
C	2.02182562	-4.56357986	0.00846524
O	1.19630033	-5.65261766	0.46916977
C	1.65595807	-4.25018231	-1.45007798
O	0.83369305	-3.08695029	-1.53087865

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C	5.28437985	-4.04942178	-1.11945993	H	2.12768150	-5.44857932	4.14123698
C	6.61706566	-3.38362737	-0.67787774	H	3.51282524	-4.17606600	2.27569063
O	6.99803961	-3.83970885	0.62402988	H	5.29200585	-5.20537867	2.87983237
C	6.50510147	-1.85202177	-0.73705321	H	3.74442326	-5.87464960	-0.26163750
O	7.79742708	-1.28769300	-0.64802072	H	1.79304886	-3.65143581	0.59514124
C	5.77951701	-1.36368273	-2.00649977	H	1.11786738	-5.12853896	-1.86744102
O	5.56982481	0.04333645	-1.81452477	H	2.57959411	-4.10257734	-2.04118668
C	4.44932835	-2.10306956	-2.19896918	H	1.29232403	-2.40087196	-2.10409708
O	4.77878959	-3.50614956	-2.32020976	H	5.45302668	-5.12620501	-1.32573120
C	3.59679864	-1.68357076	-3.41320372	H	7.40295305	-3.68837653	-1.40035463
O	2.25015101	-1.41325984	-3.03332132	H	6.26403018	-4.39017965	1.00412811
C	5.99814817	0.93121765	-2.80392060	H	5.87278338	-1.54542559	0.11663739
C	6.58379702	2.19162376	-2.12745755	H	7.68502670	-0.31123486	-0.62988628
O	7.56694557	1.79391737	-1.18568650	H	6.42864765	-1.53877604	-2.88981650
C	5.47338320	3.03025486	-1.48934271	H	3.83225381	-1.94278291	-1.29502009
O	6.04826773	4.24546198	-1.02901978	H	3.62375574	-2.51631420	-4.14928898
C	4.35855606	3.28468461	-2.51314884	H	4.03718046	-0.78768997	-3.89090079
O	3.37318102	4.06984583	-1.83931632	H	1.98081989	-0.47825315	-3.27388445
C	3.82662959	1.93831068	-3.03932927	H	6.77037136	0.46596972	-3.44943980
O	4.94471261	1.29375819	-3.69015614	H	7.03966849	2.80938508	-2.93516711
C	2.64542113	2.01199177	-4.03202431	H	7.79764611	2.58953370	-0.66541854
O	1.60148933	1.10510178	-3.69576758	H	5.03754209	2.44933990	-0.64375804
C	2.82802910	5.18862510	-2.48681491	H	5.31050977	4.79241110	-0.67684992
C	2.74885997	6.35768518	-1.47296824	H	4.77948881	3.85843910	-3.36610905
O	3.98432930	6.58029926	-0.78386740	H	3.49238422	1.32679526	-2.17897095
C	1.68459851	6.08677702	-0.40844034	H	3.03855606	1.75266861	-5.03743590
O	1.45024052	7.23943390	0.39440829	H	2.24389220	3.04180541	-4.07262493
C	0.35553984	5.67303115	-1.05493316	H	0.80444938	1.58973935	-3.33137113
O	-0.50372714	5.33418185	0.02218012	H	3.45345982	5.48302807	-3.35721273
C	0.60015207	4.48449381	-2.01595435	H	2.44221054	7.26721519	-2.03327350
O	1.54607442	4.92858234	-3.01776468	H	4.61552130	7.00635061	-1.39557346
C	-0.63611020	3.90429275	-2.72666043	H	2.02972645	5.23512857	0.21740514
O	-0.58846545	2.48131782	-2.79568483	H	2.31362308	7.49853681	0.77425850
C	-1.84002990	5.79758016	0.04292482	H	-0.05433002	6.53340254	-1.62775372
C	-2.14114038	6.20011581	1.50119505	H	1.05015667	3.66231594	-1.43480588
O	-1.22421064	7.15500014	2.00166309	H	-1.55408745	4.22421812	-2.19943266
C	-2.18636993	4.94407427	2.38914832	H	-0.66460933	4.31869502	-3.75673851
O	-2.62798527	5.26391001	3.70289367	H	-1.27196119	2.09059907	-2.17717035
C	-3.12375646	3.89043490	1.79195144	H	-1.96401714	6.66654057	-0.63456837
O	-3.04713168	2.74448990	2.63077548	H	-3.14542231	6.66867040	1.52587981
C	-2.66875178	3.58066938	0.34661899	H	-0.33534091	6.94998231	1.62644995
O	-2.73778932	4.81212202	-0.41117365	H	-1.16305588	4.50619860	2.41702728
C	-3.45964451	2.49962426	-0.40976855	H	-2.09993190	6.03989476	3.98490263
O	-2.58664405	1.60726952	-1.09629939	H	-4.15932428	4.29178109	1.77305935
C	-4.23900928	2.14035381	3.09638960	H	-1.61746091	3.24034906	0.39046772
C	-3.99360296	1.73983206	4.56535684	H	-4.12965018	3.01295527	-1.13364737
O	-3.58355643	2.82921546	5.36954162	H	-4.09113938	1.93441884	0.30136351
C	-2.97565695	0.58672483	4.62381442	H	-2.74777171	0.67899096	-0.75039399
O	-2.82120015	0.10502458	5.95269082	H	-5.08879587	2.84938811	3.02654449
C	-3.41843190	-0.56372357	3.71389208	H	-4.95216533	1.36917603	4.98137041
O	-2.41608555	-1.57274082	3.80317655	H	-3.04181331	3.43882916	4.81501238
C	-3.58336945	-0.00954071	2.27658321	H	-2.00766251	0.97534065	4.24049946
O	-4.59805488	1.02364242	2.31644090	H	-2.71666329	0.90133238	6.51461142
C	-3.96776855	-1.00927123	1.16912636	H	-4.39276184	-0.95882451	4.07339311
O	-3.21656440	-0.80558222	-0.02625758	H	-2.62070447	0.44304071	1.98535342
C	-2.80092529	-2.92854295	3.90848226	H	-5.04746593	-0.86824303	0.95093277
C	-1.86626380	-3.59559487	4.94072058	H	-3.81876412	-2.04410638	1.52802646
O	-1.81234600	-2.88473942	6.16358057	H	-2.57647441	-1.56818055	-0.15057607
C	-0.45829709	-3.79749744	4.35131841	H	-3.85578508	-3.00535328	4.24143698
O	0.35043086	-4.56858868	5.22728050	H	-2.27650147	-4.60084172	5.16606562
C	-0.52636827	-4.48348531	2.98399284	H	-1.87289045	-1.92163769	5.96147201
O	0.81288721	-4.60494517	2.51873310	H	-0.01121216	-2.79329396	4.19082625
C	-1.42135078	-3.60845848	2.06951687	H	0.25311146	-4.16126644	6.11295971
O	-2.74114561	-3.58909448	2.66476499	H	-0.98875991	-5.48805840	3.09307307
C	-1.57594591	-4.04091238	0.60101778	H	-1.00503051	-2.58171750	2.06460024
O	-1.56669900	-2.92631600	-0.29001120	H	-2.54554959	-4.57206660	0.50371483
H	0.52104416	-6.62392821	2.10867760	H	-0.76766635	-4.74319221	0.32803959
H	2.89452518	-7.15546114	2.01895027	H	-0.69094651	-2.90173881	-0.77819253

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

C	3.09074311	1.24131571	2.35273576	C	2.98896112	-1.81732251	-3.37904413
C	3.58111683	1.04923153	3.80884846	O	1.65689975	-1.57663492	-2.92106804
H	3.89554904	2.03450468	4.21491814	C	5.88126148	0.35085726	-2.60661913
C	2.67996185	-0.14134649	1.75641677	C	6.56584210	1.45513165	-1.76464308
C	3.87818979	-1.08472956	1.82273384	O	7.45275201	0.84240512	-0.84011331
H	4.70286508	-0.64145601	1.23695518	C	5.52058152	2.32807816	-1.06686999
H	3.62660519	-2.05284951	1.35098940	O	6.17984223	3.42112707	-0.44263020
C	4.78366662	0.07813828	3.85521096	C	4.46640001	2.79408334	-2.07951445
H	5.13411011	-0.04130139	4.90169897	O	3.53501854	3.61572681	-1.37451873
H	5.62542305	0.48404542	3.26050783	C	3.83359686	1.55441805	-2.73021876
C	4.36199177	-1.30400194	3.28396634	O	4.90022943	0.91768436	-3.46661752
C	3.19533653	-1.85882480	4.13441369	C	2.62480212	1.79542877	-3.64924232
H	2.87858178	-2.85229822	3.76538095	O	1.46739730	1.24327505	-3.02786623
H	3.53496839	-2.00134159	5.18045488	C	3.31295053	4.91313066	-1.86801153
C	2.39790002	0.50467919	4.65156209	C	3.12305260	5.86777384	-0.66569461
H	2.72814119	0.38458264	5.70508270	O	4.17825047	5.75738383	0.30115217
C	1.51462518	-0.70137364	2.62153608	C	1.80646019	5.56424844	0.04611839
H	1.22580369	-1.69486582	2.21605355	O	1.53370562	6.51911578	1.06703593
C	2.00411294	-0.88078132	4.08307221	C	0.64304030	5.56913041	-0.95330455
H	1.17405983	-1.28489518	4.69808887	O	-0.50344554	5.16271021	-0.22525551
C	1.18737205	1.45973252	4.58986846	C	0.94912456	4.58900788	-2.10747799
H	0.35522930	1.04901850	5.20224261	O	2.19769736	4.98495045	-2.72642517
H	1.46090316	2.44819600	5.01793368	C	-0.12815356	4.50815040	-3.20422392
C	0.30926419	0.26282563	2.52484602	O	-0.38754288	3.16333347	-3.60398720
H	-0.52400894	-0.16356241	3.11465379	C	-1.70878721	5.90470956	-0.28039232
C	1.88655964	2.20883595	2.27381260	C	-2.24746862	5.94333952	1.16365450
H	2.18567559	3.19652355	2.68861407	O	-1.33630711	6.52566780	2.07708110
C	0.72659717	1.63059607	3.12846913	C	-2.64179165	4.52132513	1.60147088
H	-0.14284725	2.32107226	3.08396232	O	-3.26645272	4.55059175	2.88012271
C	5.52419473	-2.29841239	3.19004786	C	-3.59330508	3.88845488	0.58327347
O	5.50652918	-3.42879474	3.65500447	O	-3.82175903	2.54547000	0.98119569
H	3.92469180	1.64909821	1.73836977	C	-2.94617329	3.94912156	-0.82146298
C	2.22080081	0.02906842	0.29338928	O	-2.64950446	5.32415286	-1.15201320
H	3.07591602	0.39698641	-0.31116300	C	-3.83321698	3.36344559	-1.90592825
H	1.92553359	-0.95441338	-0.12726057	O	-3.09134522	3.29173175	-3.12909814
C	1.03371743	1.00610031	0.21889275	C	-5.13730605	2.00683873	0.91495121
H	0.71490185	1.13870614	-0.83435590	C	-5.59601087	1.71814527	2.36626595
C	1.45363329	2.37248195	0.80570584	O	-5.66109747	2.90698355	3.11134541
H	0.61226202	3.09265325	0.74406147	C	-4.66554802	0.64530029	2.95521568
C	-0.12832549	0.43216149	1.05416176	O	-5.15978670	0.21174349	4.21215610
H	-0.99654970	1.11332438	0.98600723	C	-4.54778155	-0.55036163	1.99328068
H	-0.45663463	-0.54292142	0.64152337	O	-3.46369947	-1.36594605	2.47789761
H	2.29496954	2.79240487	0.21559517	C	-4.27143600	-0.18751046	0.51796733
O	6.53576496	-1.81779101	2.44501421	O	-5.15800056	0.86384263	0.09581394
H	7.02654470	-2.56850267	1.99325550	C	-4.50608498	-1.40187095	-0.39959589
O	-3.59131696	-1.49422221	-1.49613477	O	-3.59131696	-1.49422221	-1.49613477
C	-3.75454745	-2.65506217	2.95947401	C	-2.76173489	-2.93495150	4.11629444
C	-2.67152924	-1.82095592	5.00883702	O	-2.67152924	-1.82095592	5.00883702
C	-1.36552879	-3.31002609	3.59922120	C	-0.54865495	-3.82010661	4.64708039
O	-0.54865495	-3.82010661	4.64708039	C	-1.42996820	-4.33759393	2.46655101
C	-1.42996820	-4.33759393	2.46655101	O	-0.08496446	-4.52556755	2.04877396
O	-0.08496446	-4.52556755	2.04877396	C	-2.35964253	-3.78536796	1.35561460
C	-2.35964253	-3.78536796	1.35561460	O	-3.67231387	-3.63553214	1.95028995
O	-3.67231387	-3.63553214	1.95028995	C	-2.51747465	-4.64634829	0.07877800
C	-2.51747465	-4.64634829	0.07877800	O	-2.45329684	-3.88894701	-1.12342739
O	-2.45329684	-3.88894701	-1.12342739	H	-0.39625742	-6.57830804	1.91246968
H	-0.39625742	-6.57830804	1.91246968	H	1.95425648	-7.15369254	2.11189945
H	1.95425648	-7.15369254	2.11189945	H	1.13969977	-5.08092015	3.86314540
H	1.13969977	-5.08092015	3.86314540	H	2.61429506	-4.17885184	1.91880255
H	2.61429506	-4.17885184	1.91880255	H	4.01935561	-5.69477689	3.08047843
H	4.01935561	-5.69477689	3.08047843	H	3.00235185	-6.33951623	-0.23275858
H	3.00235185	-6.33951623	-0.23275858	H	1.14586194	-3.89615339	0.09971015
H	1.14586194	-3.89615339	0.09971015	H	0.62460328	-5.74600669	-2.18384167
H	0.62460328	-5.74600669	-2.18384167	H	1.96416592	-4.56881780	-2.40731350
H	1.96416592	-4.56881780	-2.40731350	H	0.53591345	-2.90714218	-2.30667065
H	0.53591345	-2.90714218	-2.30667065	H	4.43528115	-5.70234910	-1.82929502

10a_beta-CD_S:

C	0.34176178	-5.80455878	1.61929927	O	-2.67152924	-1.82095592	5.00883702
C	1.70651881	-6.08717914	2.28428931	C	-1.36552879	-3.31002609	3.59922120
O	1.67309600	-5.89109125	3.68720853	O	-0.54865495	-3.82010661	4.64708039
C	2.81504210	-5.23735784	1.64004709	C	-1.42996820	-4.33759393	2.46655101
O	4.09523855	-5.63739455	2.10534715	O	-0.08496446	-4.52556755	2.04877396
C	2.78131511	-5.30429555	0.10664425	C	-2.35964253	-3.78536796	1.35561460
O	3.79108314	-4.40809784	-0.32902912	O	-3.67231387	-3.63553214	1.95028995
C	1.35363705	-4.89275496	-0.33915658	C	-2.51747465	-4.64634829	0.07877800
O	0.43865619	-5.86415974	0.21807322	O	-2.45329684	-3.88894701	-1.12342739
C	1.04056401	-4.77810502	-1.83927013	H	-0.39625742	-6.57830804	1.91246968
O	0.07070231	-3.76191102	-2.09440664	H	1.95425648	-7.15369254	2.11189945
C	4.50316253	-4.63715511	-1.52824745	H	1.13969977	-5.08092015	3.86314540
C	5.97640186	-4.25692951	-1.23658324	H	2.61429506	-4.17885184	1.91880255
O	6.45929522	-5.00072439	-0.14067753	H	4.01935561	-5.69477689	3.08047843
C	6.08002453	-2.73116075	-1.04910657	H	3.00235185	-6.33951623	-0.23275858
O	7.43421431	-2.32880124	-1.06081948	H	1.14586194	-3.89615339	0.09971015
C	5.29538693	-1.96629478	-2.13952972	H	0.62460328	-5.74600669	-2.18384167
O	5.32013720	-0.58904238	-1.73922686	H	1.96416592	-4.56881780	-2.40731350
C	3.85347524	-2.48113159	-2.29108707	H	0.53591345	-2.90714218	-2.30667065
O	3.95530162	-3.88896012	-2.59419360	H	4.43528115	-5.70234910	-1.82929502

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H	6.58863139	-4.53851907	-2.11644664	H	-0.98746946	-0.84275337	1.72302066
H	5.78417149	-4.94112836	0.57228995	C	0.22815370	0.54088914	0.54865895
H	5.59823752	-2.49710416	-0.07438793	C	0.78936711	1.96701155	0.70800497
H	7.44986320	-1.37051258	-0.84502318	H	1.37956495	2.22176087	-0.19228957
H	5.82476347	-2.09352414	-3.10701734	H	-0.03838217	2.69811181	0.77857581
H	3.32788058	-2.34364455	-1.32787920	C	0.94304074	1.64115757	3.24685108
H	2.96186739	-2.50139867	-4.25421368	H	0.09013269	2.33776528	3.39905250
H	3.46741540	-0.87676477	-3.70492520	C	2.89374090	1.07490245	1.76777563
H	1.46318796	-0.60176968	-2.92920935	H	3.44312212	1.36745348	0.84975499
H	6.62635332	-0.12096857	-3.27808610	C	1.69958368	2.03711818	1.95115620
H	7.12466715	2.10493436	-2.47636132	H	2.08755354	3.07143689	2.07033018
H	7.73243144	1.53764221	-0.21152660	C	1.89043684	1.69373295	4.46084114
H	5.00753453	1.69779291	-0.30869726	H	2.27418996	2.72732535	4.59774845
H	5.47498509	3.95056929	-0.00609630	H	1.33427676	1.42212082	5.38366873
H	4.96237163	3.38450238	-2.87810359	C	3.86353440	1.11495502	2.97476371
H	3.48846017	0.87320633	-1.92916665	H	4.24545313	2.15267235	3.09060415
H	2.83222711	1.30695157	-4.62781365	C	2.54971231	-0.73203838	4.07543726
H	2.48253284	2.87929442	-3.83240648	H	1.98871276	-1.03073613	4.98826539
H	0.68831719	1.84769618	-3.20294693	C	3.06876037	0.72209687	4.25024334
H	4.17581286	5.24965175	-2.48142587	H	3.74715057	0.76176316	5.12866659
H	3.06702544	6.90358503	-1.06288126	C	-0.75589921	0.42897648	-0.61745962
H	4.93072410	6.30311849	0.00293658	O	-1.16376185	1.36109601	-1.29370695
H	1.87507505	4.54245672	0.47257135	H	1.20307996	-1.80375685	2.74016307
H	2.31382694	6.52480063	1.65751367	C	3.56479297	-1.31498020	1.35781326
H	0.51081786	6.59655440	-1.35777885	H	3.21504280	-2.34532200	1.15981741
H	1.05365446	3.57908921	-1.67466582	H	4.11239199	-0.98023656	0.45538399
H	-1.06858946	4.97190282	-2.84869673	C	4.50670107	-1.28954906	2.57734586
H	0.23859976	5.08447092	-4.08005535	H	5.34827481	-1.99270521	2.40933826
H	-1.28987715	2.93190778	-3.26575025	C	3.72474691	-1.70624808	3.84437732
H	-1.52297919	6.93068668	-0.65825112	H	4.39911504	-1.70149602	4.72726109
H	-3.16216932	6.56859582	1.17228787	C	5.04609141	0.14761266	2.75381762
H	-0.42226073	6.27176936	1.80480849	H	5.73807629	0.19623931	3.62166968
H	-1.71947796	3.90190331	1.63848635	H	5.62260566	0.44530105	1.85116207
H	-2.71951836	5.13791905	3.44207532	H	3.33808371	-2.74204678	3.73021485
H	-4.54231916	4.46508466	0.58635718	O	-1.18169841	-0.83372288	-0.76500114
H	-2.01111403	3.36329470	-0.79882289	H	-2.07853375	-0.89320298	-1.24900203
H	-4.73392493	4.00647644	-2.03783105				
H	-4.14782622	2.35323005	-1.57460718				
H	-3.56091555	2.69543872	-3.74104094				
H	-5.83316684	2.73067480	0.44600691				
H	-6.62414779	1.30598820	2.32909704				
H	-4.76763842	3.32352431	3.12875805				
H	-3.65413425	1.10202140	3.05086232				
H	-4.50243051	-0.40364362	4.59834615				
H	-5.50262421	-1.11376924	2.05246903				
H	-3.22470268	0.15767900	0.44386280				
H	-5.54669298	-1.31947351	-0.78342225				
H	-4.43961007	-2.32196755	0.21235267				
H	-3.25922469	-2.44456069	-1.49488002				
H	-4.79527434	-2.70437419	3.33718772				
H	-3.14863380	-3.78122403	4.71425931				
H	-2.38630634	-1.06573539	4.45022669				
H	-0.90598971	-2.39548793	3.16684966				
H	-0.60252758	-3.17746694	5.38339101				
H	-1.85281285	-5.28898229	2.85529546				
H	-1.97604584	-2.79739241	1.03186086				
H	-3.51324743	-5.13117634	0.12719122				
H	-1.74577687	-5.43749702	0.05064957				
H	-1.50043383	-3.81802511	-1.43695146				
C	1.58630889	-0.76808268	2.86471724				
C	0.39389141	0.20497727	3.05711455				
H	-0.16995111	-0.09324153	3.97079448				
C	2.36386472	-0.37790416	1.56985225				
C	1.41044109	-0.44360187	0.36522729				
H	1.02457973	-1.47523551	0.24750810				
H	1.95321289	-0.19581327	-0.56743119				
C	-0.54709324	0.16147757	1.84408758				
H	-1.38848718	0.87070233	1.98740161				

10a_gamma-CD_P:

C	4.02535341	-5.76202674	0.18699939
C	4.16451352	-6.03518338	-1.32911873
C	2.89403751	-5.54436654	-2.04363099
C	1.65262954	-6.14384750	-1.35232458
C	1.61446706	-5.89309375	0.16211139
C	0.51345395	-6.67160173	0.88690729
O	5.36926931	-5.49119288	-1.80309564
O	2.93026720	-5.91623427	-3.40077775
O	0.50757339	-5.53678412	-1.95020966
O	2.86254853	-6.35269560	0.74891650
O	0.64981615	-8.07187786	0.71486122
C	-0.39690425	-6.32124431	-2.68554540
C	-0.78049420	-5.53428318	-3.95518681
C	-1.49924607	-4.23928077	-3.55749034
C	-2.68959505	-4.57601715	-2.66170190
C	-2.23991302	-5.42488198	-1.45858826
C	-3.39975161	-5.88990423	-0.58245962
O	0.39104531	-5.25980124	-4.71560653
O	-1.85321179	-3.49447989	-4.71884390
O	-3.23907383	-3.34102413	-2.21312609
O	-1.56610064	-6.61050772	-1.93795146
O	-4.41317423	-6.56260726	-1.32173798
C	-4.64058478	-3.21159960	-2.17585311
C	-5.14677420	-2.52544020	-3.45888197
C	-4.58461789	-1.10803696	-3.57269735
C	-4.80839451	-0.30663565	-2.27945757
C	-4.36781765	-1.11855462	-1.04993935
C	-4.73063958	-0.49813166	0.29591436
O	-4.76104393	-3.29435822	-4.60444475

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O	-5.20266594	-0.52031140	-4.69980303	H	1.55898468	-8.29557955	0.99785721
O	-4.00510289	0.88155898	-2.37631634	H	0.04801208	-7.30059745	-2.94968692
O	-4.99452734	-2.41662525	-1.06685003	H	-1.48252863	-6.16783497	-4.54306993
O	-4.11821552	-1.19468737	1.36638837	H	-0.78824609	-3.63537327	-2.96510634
C	-4.59003338	2.15091024	-2.29681645	H	-3.43775458	-5.14960220	-3.24405024
C	-4.28710731	2.93033332	-3.59955180	H	-1.55927113	-4.81276882	-0.84047674
C	-2.78266974	3.18072694	-3.70187598	H	-3.86530450	-5.00642389	-0.11041820
C	-2.34598504	3.94895145	-2.44833537	H	-2.98491851	-6.53322696	0.22790990
C	-2.66543115	3.11528845	-1.19536060	H	0.15497209	-4.53877914	-5.33494588
C	-2.31283048	3.82584349	0.11078026	H	-2.83874206	-3.42910440	-4.75641637
O	-4.77627046	2.21809300	-4.72790768	H	-3.96618128	-7.28572638	-1.80566914
O	-2.55481723	3.89456021	-4.91590669	H	-5.13161191	-4.19456120	-2.03233576
O	-0.95537049	4.26028003	-2.53311198	H	-6.25540336	-2.46447278	-3.39994500
O	-4.09414474	2.87867808	-1.18137795	H	-3.48319175	-1.20333646	-3.71030777
O	-2.85898658	5.14302863	0.18043461	H	-5.88471638	-0.04343806	-2.20216018
C	-0.70274179	5.54375311	-3.09562688	H	-3.26865052	-1.23924196	-1.09837721
C	0.61552995	5.45885471	-3.88028105	H	-4.37138587	0.54949460	0.32276554
C	1.83991773	5.47951132	-2.95487991	H	-5.84435709	-0.48953360	0.38879432
C	1.74666885	6.57211507	-1.87064221	H	-5.00274782	-2.74268656	-5.37857808
C	0.38036835	6.43564765	-1.13921101	H	-4.92356834	0.42773362	-4.75669613
C	-0.01568833	7.46773090	-0.06149973	H	-4.12834451	-2.14683247	1.13632056
O	0.63265833	4.31060951	-4.73619024	H	-5.68541224	2.08089027	-2.14006677
O	3.03089265	5.67321129	-3.70167813	H	-4.79910495	3.91508243	-3.52896578
O	2.89439642	6.31203136	-1.06404644	H	-2.25892581	2.20029953	-3.72290068
O	-0.66911273	6.54630971	-2.12519840	H	-2.92661084	4.88696759	-2.35952850
O	-0.80483120	6.88509466	0.96648558	H	-2.12926961	2.14767170	-1.23177541
C	3.22400556	7.13055336	0.03092335	H	-1.21900322	3.93829487	0.20113401
C	4.75754286	7.05077880	0.17555164	H	-2.65854946	3.19810559	0.96143110
C	5.18440411	5.67703928	0.72165830	H	-4.33318342	2.61170872	-5.50963051
C	4.36982037	5.25957900	1.95308466	H	-1.58836373	3.91143437	-5.09349074
C	2.87982174	5.33560415	1.56180315	H	-3.83204203	5.07768543	0.12864460
C	1.84981913	4.87871448	2.59541955	H	-1.52384418	5.82360400	-3.77976169
O	5.42808985	7.33080498	-1.04316410	H	0.67801980	6.33927802	-4.54680577
O	6.57230993	5.70652779	1.05023025	H	1.87189114	4.50844373	-2.40339942
O	4.74859535	3.93133629	2.29149402	H	1.82753142	7.57860287	-2.33870118
O	2.59049632	6.70771396	1.21729430	H	0.36075000	5.43341939	-0.66802639
O	0.58235110	4.67147684	2.00455268	H	-0.55890071	8.29140223	-0.57631186
C	5.28979614	3.63598710	3.56935164	H	0.85659467	7.89297525	0.45050938
C	6.66086432	2.96823914	3.36094903	H	0.54530832	3.53063051	-4.14678022
C	6.44933444	1.65527418	2.58893227	H	2.99587994	5.03697056	-4.44464466
C	5.50791000	0.74404997	3.38070065	H	-1.61232771	6.45528815	0.58676759
C	4.18802709	1.50124598	3.68737145	H	2.90734575	8.17907930	-0.14556054
C	3.27538205	0.73987830	4.66414948	H	5.07548793	7.82079373	0.90424917
O	7.62783999	3.77441150	2.72423172	H	4.99328455	4.91577859	-0.06749848
O	7.72929046	1.03853083	2.38079575	H	4.57385132	5.95806079	2.79236587
O	5.15625100	-0.44197793	2.66119919	H	2.73201206	4.70000048	0.66921213
O	4.44870154	2.77705474	4.29945229	H	1.81437891	5.61893540	3.42969990
O	2.70898754	-0.41948436	4.09422186	H	2.18925096	3.91051948	3.01155528
C	6.13806095	-1.48351835	2.59488067	H	4.95256227	6.81838300	-1.73565615
C	6.54259475	-1.73776211	1.11534582	H	7.03569637	6.08595824	0.27424997
C	5.42098894	-2.45688429	0.36383603	H	0.17390225	5.54196443	1.75595156
C	5.02775251	-3.72561005	1.11651932	H	5.39016402	4.55908650	4.17515713
C	4.57564071	-3.32630779	2.53822110	H	7.06628763	2.71902216	4.36246497
C	4.15057502	-4.49387483	3.45288155	H	5.97826754	1.87746563	1.60866414
O	6.84227373	-0.56477610	0.38731265	H	5.99800667	0.47187306	4.34228778
O	5.82369067	-2.78070114	-0.96254072	H	3.64762052	1.64747556	2.73135079
O	3.98098743	-4.36251044	0.39682795	H	2.44354269	1.41434352	4.94726732
O	5.66335246	-2.65322528	3.20603807	H	3.85939915	0.51771559	5.59132046
O	2.84670210	-4.95655820	3.19540657	H	7.20037008	4.32325293	2.01473007
H	4.88125860	-6.21433326	0.72606855	H	8.34069794	1.79339808	2.21201396
H	4.23364227	-7.13238003	-1.47498263	H	3.42705637	-0.89003058	3.62387274
H	2.84004624	-4.43558903	-1.91997094	H	7.02873114	-1.18402373	3.17897706
H	1.64598526	-7.23979344	-1.51849821	H	7.42149195	-2.42479829	1.14914882
H	1.49709517	-4.80724963	0.35279468	H	4.54121861	-1.78661048	0.33894801
H	-0.46512107	-6.38588425	0.46467331	H	5.91164891	-4.39482770	1.18710325
H	0.53113301	-6.37674890	1.96323790	H	3.69840907	-2.65402916	2.44634369
H	5.36259750	-4.51745090	-1.64898627	H	4.16717798	-4.09640213	4.48780843
H	2.11179935	-5.57040228	-3.82921468	H	4.91873470	-5.30451621	3.39665832

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H	7.39065799	0.02405713	0.96767275	O	0.39936291	-5.22324386	-4.74266036
H	6.20117388	-1.96586768	-1.35085581	O	-1.85775379	-3.47510539	-4.70150716
H	2.85714673	-5.51805568	2.38663404	O	-3.22430427	-3.36978369	-2.18119446
C	2.16701785	-1.03056469	-0.74444943	O	-1.52166087	-6.62756119	-1.96634988
C	2.01886851	-0.62919545	0.74368534	O	-4.36743644	-6.60890339	-1.32685350
H	3.01232530	-0.63350906	1.23209118	C	-4.62609215	-3.24884573	-2.13513792
C	0.75623295	-1.04961152	-1.41668356	C	-5.14573416	-2.55877257	-3.41046273
C	-0.17381419	-2.02054333	-0.65841850	C	-4.59124432	-1.13815317	-3.52180935
H	0.23533740	-3.04841060	-0.72273083	C	-4.80627544	-0.34351165	-2.22286885
H	-1.16911549	-2.04690399	-1.14227148	C	-4.35348793	-1.16057348	-1.00110647
C	1.09241396	-1.61194989	1.48672279	C	-4.70733746	-0.54998296	0.35174070
H	1.01722943	-1.31967601	2.54898931	O	-4.76605350	-3.31918858	-4.56378437
H	1.51693685	-2.63665483	1.45119396	O	-5.22186848	-0.54849070	-4.64090701
C	-0.31485094	-1.60634744	0.82425029	O	-4.00672987	0.84738032	-2.31963665
C	-0.88848321	-0.15837956	0.90138000	O	-4.97639123	-2.46064224	-1.02021472
H	-1.89866524	-0.13916211	0.45130200	O	-4.08670509	-1.25483879	1.41199436
H	-0.99476126	0.13927675	1.96195657	C	-4.59412461	2.11525598	-2.23248714
C	1.45355723	0.81053338	0.81320155	C	-4.30774391	2.89827591	-3.53716380
H	1.36047352	1.11020690	1.87630294	C	-2.80486444	3.14983240	-3.65682279
C	0.18287687	0.39935321	-1.32508471	C	-2.35532125	3.91836253	-2.40834124
H	-0.82400616	0.39627215	-1.79926083	C	-2.65949717	3.08458034	-1.15156232
C	0.04878732	0.80787806	0.16333907	C	-2.29421301	3.79857330	0.14941502
H	-0.36423092	1.83470137	0.22726020	O	-4.80966531	2.18950937	-4.66214400
C	2.36695855	1.79880189	0.06555775	O	-2.59140734	3.86441532	-4.87299315
H	1.92788129	2.81528858	0.13369992	O	-0.96641815	4.23208503	-2.50805561
H	3.37102408	1.83543778	0.53554778	O	-4.08728896	2.84316544	-1.12177073
C	1.10567314	1.378777854	-2.09198254	O	-2.83779877	5.11689595	0.22072580
H	0.66765640	2.39701189	-2.02428945	C	-0.72089789	5.51596668	-3.07320669
C	3.09640232	-0.04961130	-1.50870042	C	0.59083153	5.43116993	-3.86872961
H	4.09757801	-0.04812418	-1.02936028	C	1.82173582	5.44826865	-2.95197400
C	2.49859281	1.37918054	-1.40911071	C	1.73853727	6.54045641	-1.86669777
H	3.16413990	2.09193349	-1.94528282	C	0.37722250	6.40772251	-1.12564296
C	-1.27271421	-2.53852831	1.55927203	C	-0.00744232	7.44136118	-0.04535567
O	-1.95858689	-3.41291565	1.05374491	O	0.59978925	4.28400516	-4.72602688
H	2.59169657	-2.05528435	-0.80663932	O	3.00837950	5.63935767	-3.70641862
C	0.89736237	-1.45572674	-2.90089848	O	2.88996549	6.27631783	-1.06739001
H	1.30628818	-2.48629693	-2.96462762	O	-0.67964422	6.51895254	-2.10351012
H	-0.10229856	-1.47001153	-3.38363754	O	-0.78410192	6.86062824	0.99310238
C	1.82723176	-0.47500798	-3.64838973	C	3.23736824	7.10209663	0.01647245
H	1.91535348	-0.78361980	-4.71042756	C	4.77257266	7.01510424	0.14292582
C	3.22354866	-0.48264155	-2.98363085	C	5.19942800	5.64413367	0.69704058
H	3.90712070	0.20689233	-3.52484514	C	4.39656604	5.24224403	1.94133257
C	1.23100320	0.95091250	-3.56923633	C	2.90284959	5.32167153	1.56596658
H	1.88561998	1.66321566	-4.11975083	C	1.88413280	4.87461049	2.61499812
H	0.22950883	0.96868719	-4.05455678	O	5.42922632	7.27989177	-1.08670112
H	3.66743782	-1.49962939	-3.03457334	O	6.59106393	5.66947585	1.00972315
O	-1.31247553	-2.28030449	2.88719946	O	4.77213104	3.91539004	2.28798647
H	-1.98604641	-2.88272894	3.27379957	O	2.61546017	6.69236049	1.21380077
O	0.61111433	4.65842091	2.03962661	O	5.30880648	3.62487600	3.56868937
C	6.68361290	2.96318338	3.36580430	C	6.47955107	1.65022841	2.59189767

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C	4.07827194	-5.75239030	0.12738951	C	5.3847330	0.73381530	3.37803445
C	4.20618019	-6.00915408	-1.39263923	C	4.21514563	1.48481379	3.68616795
C	2.92685400	-5.51972249	-2.09239333	C	3.31008563	0.71916033	4.66681341
C	1.69517312	-6.13445747	-1.39708064	O	7.64804814	3.77473829	2.73178919
C	1.66769097	-5.89568649	0.11944499	O	7.76227319	1.03789314	2.38712353
C	0.57536192	-6.68327964	0.84709562	O	5.18947875	-0.44947517	2.65236594
O	5.40330020	-5.45297760	-1.87153618	O	4.46872032	2.76292175	4.29649453
O	2.95572061	-5.87819925	-3.45343348	O	2.75699320	-0.45039800	4.10447121
O	0.54068675	-5.53202553	-1.98123399	C	6.17341873	-1.48834567	2.57915807
O	2.92260462	-6.35541579	0.69211610	C	6.58112932	-1.72921878	1.09831180
O	0.71659584	-8.08178612	0.66428139	C	5.46268997	-2.44562012	0.33932236
C	-0.36109864	-6.31718579	-2.71918386	C	5.07205153	-3.72210378	1.08035665
C	-0.76301066	-5.51829124	-3.97578156	C	4.61562758	-3.33516558	2.50423338
C	-1.48941494	-4.23503314	-3.55432075	C	4.19253072	-4.50958881	3.41063953
C	-2.66971900	-4.59346864	-2.65374053	O	6.87759407	-0.54905752	0.38065758
C	-2.20291066	-5.45473466	-1.46630549	O	5.86845576	-2.75673833	-0.98907094

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O	4.02905731	-4.35571138	0.35209863	H	2.47039011	1.38580568	4.94580062
O	5.69996213	-2.66401766	3.17972321	H	3.89692297	0.50940894	5.59516596
O	2.89302872	-4.97920421	3.14372353	H	7.22145222	4.30876540	2.01056471
H	4.94083962	-6.20620952	0.65453009	H	8.37181159	1.79518045	2.22230423
H	4.28025956	-7.10445745	-1.54996553	H	3.47944063	-0.91473916	3.63451176
H	2.86587706	-4.41271453	-1.95743281	H	7.06197382	-1.19209462	3.16768269
H	1.69573711	-7.22900691	-1.57177695	H	7.46257323	-2.41313025	1.12759102
H	1.54864576	-4.81198678	0.32025638	H	4.58062719	-1.77802933	0.31939730
H	-0.40729172	-6.39841089	0.43398398	H	5.95763241	-4.38952291	1.14767040
H	0.59941162	-6.39569560	1.92520960	H	3.73732160	-2.66430105	2.41484937
H	5.39450073	-4.48188754	-1.70145674	H	4.20116691	-4.11718667	4.44755714
H	2.13202871	-5.53389259	-3.87287845	H	4.96621008	-5.31499484	3.35489246
H	1.62996015	-8.30249655	0.93587721	H	7.42491693	0.03558219	0.96631659
H	0.09175375	-7.28849617	-2.99907804	H	6.24057512	-1.93628335	-1.37067598
H	-1.46469849	-6.15083938	-4.56520550	H	2.91237880	-5.53766493	2.33292868
H	-0.77831712	-3.63484356	-2.95914042	C	2.18447333	-1.04541342	-0.73917069
H	-3.41877633	-5.16421406	-3.23748703	C	2.04204294	-0.65082794	0.75135778
H	-1.52339756	-4.84402653	0.84564411	H	3.03798746	-0.65039942	1.23482310
H	-3.81752814	-5.06844153	-0.09686596	C	0.76996326	-1.07074532	-1.40358582
H	-2.92399454	-6.59461962	0.20894955	C	-0.14999387	-2.05012989	-0.64408694
H	0.15237543	-4.49320793	-5.34713672	H	0.26367140	-3.07562513	-0.71567835
H	-2.84437667	-3.42629377	-4.73665921	H	-1.14816922	-2.07904640	-1.12160646
H	-3.92105751	-7.32228210	-1.82556730	C	1.12579184	-1.64215662	1.49578134
H	-5.11078519	-4.23519108	-1.99315949	H	1.05475568	-1.35355395	2.55942999
H	-6.25416333	-2.50321030	-3.34210597	H	1.55613692	-2.66422174	1.45552921
H	-3.49086244	-1.22799984	-3.66938672	C	-0.28511299	-1.64332340	0.84107530
H	-5.88257381	-0.08333075	-2.13544412	C	-0.86762103	-0.19961028	0.92790313
H	-3.25441206	-1.27800278	-1.05865906	H	-1.88075646	-0.18471313	0.48431705
H	-4.34757205	0.49745396	0.38400106	H	-0.96866777	0.09324745	1.99039187
H	-5.82036523	-0.54266405	0.45345348	C	1.46780281	0.78488359	0.82967206
H	-5.02117785	-2.76549486	-5.33214664	H	1.37899822	1.08001952	1.89448921
H	-4.94676148	0.40081771	-4.69657057	C	0.18760040	0.37392617	-1.30298040
H	-4.10069492	-2.20516295	1.17500158	H	-0.82185348	0.36599231	-1.77181869
H	-5.68764126	2.04210942	-2.06388529	C	0.05926606	0.77540863	0.18790108
H	-4.81957249	3.88248850	-3.45761513	H	-0.36003456	1.79923091	0.25826130
H	-2.28070654	2.16975985	-3.68435149	C	2.37048923	1.78213200	0.08081664
H	-2.93657396	4.85547679	-2.31346446	H	1.92497991	2.79543115	0.15565534
H	-2.12117255	2.11836938	-1.19260978	H	3.37702988	1.82353323	0.54514435
H	-1.19934060	3.90956522	0.22917901	C	1.09982833	1.36232128	-2.07112067
H	-2.63276241	3.17409398	1.00517947	H	0.65589518	2.37755142	-1.99797626
H	-4.37661570	2.58707094	-5.44757551	C	3.10306621	-0.05532369	-1.50484722
H	-1.62716942	3.88129221	-5.06202857	H	4.10690963	-0.04865793	-1.03127009
H	-3.81154129	5.05332278	0.18246830	C	2.49655032	1.36910539	-1.39615270
H	-1.54850663	5.79408809	-3.75015845	H	3.15438639	2.08821088	-1.93331643
H	0.64912998	6.31237785	-4.53467777	C	-1.23170888	-2.58720300	1.57622808
H	1.85493807	4.47703660	-2.40103089	O	-1.90950871	-3.46736737	1.07125777
H	1.81923638	7.54683985	-2.33473825	H	2.61547613	-2.06708601	-0.80748308
H	0.35975792	5.40602271	-0.65356294	C	0.90517305	-1.46978299	-2.89017539
H	-0.55765935	8.26311656	-0.55566969	H	1.31886364	-2.49782814	-2.96077343
H	0.87060826	7.86883227	0.45516669	H	-0.09695623	-1.48624043	-3.36752849
H	0.51623197	3.50363277	-4.13672806	C	1.82509920	-0.48089217	-3.63881061
H	2.96746775	5.00321351	-4.44919157	H	1.90906039	-0.78491111	-4.70252376
H	-1.59406495	6.42652931	0.62320929	C	3.22501837	-0.48177239	-2.98205029
H	2.92421872	8.15097742	-0.16502416	H	3.90044542	0.21499871	-3.52430028
H	5.10403959	7.79063015	0.85991630	C	1.22007371	0.94069361	-3.55057487
H	4.99576870	4.87666458	-0.08290531	H	1.86733556	1.65908051	-4.10172369
H	4.61335567	5.94754156	2.77154845	H	0.21609378	0.95406191	-4.03069409
H	2.74267689	4.67944102	0.68021134	H	3.67613893	-1.49518717	-3.03988757
H	1.85632525	5.62363847	3.44209747	O	-1.26932954	-2.33250185	2.90566892
H	2.23060408	3.91149445	3.03721335	H	-1.93425660	-2.94388125	3.29329383
H	4.94255677	6.76409737	-1.76897323				
H	7.04864992	6.03751926	0.22501963				
H	0.19956877	5.52568612	1.78468623				
H	5.40200777	4.54900402	4.17409638				
H	7.08771762	2.71574297	4.36830133				
H	6.01157839	1.87260086	1.61029885				
H	6.02832093	0.45809887	4.33876611				
H	3.67202070	1.62629191	2.73105775				

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C	5.99701433	-1.91689075	-1.91383445
C	7.18841443	-1.15192612	-1.30443146
O	8.05842789	-1.98491567	-0.56528729
C	6.65973511	0.01072875	-0.44634728
O	7.72836647	0.84374035	-0.01163225

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

C	5.67227625	0.86425488	-1.24248068	C	3.32361803	-3.92990858	-1.04716314
O	5.19714129	1.88863196	-0.36638324	O	2.92105298	-5.31521248	-1.06496998
C	4.53491102	-0.03124355	-1.78816509	C	2.69612687	-3.22865579	-2.26109503
O	5.14053627	-1.04620948	-2.62311315	O	1.44692633	-2.62030911	-1.92746420
C	3.44442466	0.68311172	-2.60499427	H	6.34921744	-2.66841564	-2.64912943
O	2.13769749	0.20301885	-2.28321084	H	7.78014723	-0.71696130	-2.13497736
C	5.27900558	3.23727217	-0.80845399	H	7.51836697	-2.66885461	-0.10122111
C	5.79178734	4.10774299	0.36384782	H	6.12073378	-0.41754478	0.42714183
O	6.94073243	3.54742418	0.97051302	H	8.40430811	0.24657990	0.37117824
C	4.68194009	4.39209500	1.38937935	H	6.20785994	1.31862450	-2.10244718
O	5.10319691	5.46052029	2.20174990	H	4.04070375	-0.52317979	-0.93467651
C	3.31164744	4.68495919	0.74585637	H	3.65532591	0.50284944	-3.68112634
O	2.37764997	4.64872989	1.83380336	H	3.50099284	1.77310009	-2.42120284
C	2.97680181	3.63883814	-0.33335723	H	1.62428419	0.96957324	-1.91401221
O	4.04246134	3.68022047	-1.30811916	H	5.98910960	3.30978154	-1.65612613
C	1.64842260	3.83130779	-1.08517562	H	6.07126790	5.09145108	-0.06934601
O	0.98958553	2.59253520	-1.35167307	H	7.01410335	2.59485184	0.72688670
C	1.51258193	5.73744856	2.02399894	H	4.52234718	3.47172193	1.99141022
C	1.31874232	5.97018843	3.54981010	H	4.49728779	5.50482267	2.96950955
O	2.55614941	6.11483956	4.21352016	H	3.33343575	5.69369752	0.28476972
C	0.41694455	4.89253085	4.17663835	H	2.95621208	2.64118691	0.14662885
O	0.04099063	5.30454800	5.47097241	H	1.87826908	4.34219138	-2.04468126
C	-0.82038472	4.62897130	3.29896673	H	0.98873634	4.49548322	-0.49631837
O	-1.47554413	3.49382695	3.86803785	H	0.12530046	2.58616968	-0.85978017
C	-0.41638907	4.35670930	1.84198913	H	1.93350508	6.65498457	1.56849590
O	0.26582657	5.52978362	1.36629937	H	0.78590938	6.93634941	3.65493959
C	-1.58113612	4.02447313	0.88622574	H	2.91048596	5.22686499	4.43628898
O	-1.33566780	2.85701621	0.10228456	H	0.99273927	3.93319369	4.20509553
C	-2.84943052	3.50623354	4.15344472	H	-0.72221534	4.74923252	5.77118724
C	-3.02850599	3.09867591	5.63120993	H	-1.48213115	5.52009129	3.34028451
O	-2.31343686	4.03834182	6.40727953	H	0.27662598	3.49252147	1.82866062
C	-2.54682710	1.65352440	5.82136050	H	-1.71595707	4.88738992	0.20286423
O	-2.80773411	1.23876481	7.16701462	H	-2.51607137	3.89041221	1.46523440
C	-3.25076166	0.72486204	4.80695926	H	-1.86743727	2.09781803	0.44883216
O	-2.70829785	-0.57253109	4.98870426	H	-3.29114386	4.50709192	3.97259628
C	-3.01807925	1.26221322	3.37757789	H	-4.11524671	3.13526333	5.86969655
O	-3.55277239	2.60392378	3.31871819	H	-2.17779545	3.71693369	7.32318150
C	-3.66104592	0.48419468	2.22738414	H	-1.45825789	1.61905083	5.61488576
O	-3.46694102	1.19381330	0.99641351	H	-1.96122774	0.93221281	7.56216129
C	-3.56619162	-1.68369093	5.19286307	H	-4.34327389	0.72726093	5.01478119
C	-2.89817444	-2.53267600	6.30344407	H	-1.93039916	1.30401476	3.18656110
O	-2.68287033	-1.73956736	7.47944640	H	-3.18506685	-0.50398285	2.10025588
C	-1.58407277	-3.11702577	5.75053609	H	-4.74584838	0.32860816	2.42138184
O	-0.87805905	-3.89230319	6.70701551	H	-3.97018328	2.02894267	1.07714314
C	-1.94930899	-3.95453217	4.50338876	H	-4.57034583	-1.33978538	5.52285384
O	-0.75460143	-4.54100726	4.01641957	H	-3.57906177	-3.36542957	6.57194363
C	-2.58377121	-3.00352365	3.45838272	H	-3.07336344	-0.84430947	7.33277706
O	-3.78054660	-2.41842673	4.02698487	H	-0.95070001	-2.27336770	5.41497065
C	-2.94176584	-3.58951866	2.07955137	H	-0.16911325	-3.31264777	7.06540988
O	-2.55790135	-2.69873405	1.04677967	H	-2.67786066	-4.74493660	4.78589469
C	-0.74205615	-5.90340710	3.63065782	H	-1.84567354	-2.20575484	3.26817407
C	0.57387659	-6.50007169	4.16871572	H	-4.04398885	-3.74300181	2.06261497
O	0.72431774	-6.30777332	5.56117298	H	-2.46015024	-4.57837401	1.96101276
C	1.77276687	-5.92936035	3.38800319	H	-1.87075863	-3.13842148	0.48116197
O	2.97126278	-6.61517501	3.73339323	H	-1.61358748	-6.43767060	4.05988700
C	1.54846173	-6.05300584	1.87953137	H	0.55040063	-7.59396361	3.98864412
O	2.66133612	-5.42803902	1.25103694	H	0.33850000	-5.42704090	5.78974073
C	0.21084222	-5.37376391	1.51137002	H	1.86114500	-4.84564908	3.62913350
O	-0.83827564	-6.06121663	2.23180264	H	3.00428785	-6.63059133	4.71241887
C	-0.15323212	-5.33384244	0.01045508	H	1.50446387	-7.12960852	1.60806513
O	-0.60583894	-4.04886082	-0.41106516	H	0.25161960	-4.33045354	1.86372641
C	3.24919999	-6.02114021	0.11106528	H	-0.97597702	-6.05911836	-0.15434523
C	4.77324522	-6.03943173	0.34948934	H	0.71213806	-5.64205911	-0.60513368
O	5.13051383	-6.69606679	1.54954765	H	0.12750838	-3.54069496	-0.84324260
C	5.31752306	-4.60337633	0.31365411	H	2.87002047	-7.05245092	-0.03571513
O	6.73894479	-4.59392146	0.36933547	H	5.24559926	-6.60322659	-0.47970757
C	4.86553768	-3.87666637	-0.95488050	H	4.48495927	-6.43783025	2.25132674
O	5.33289338	-2.53932461	-0.83509556	H	4.88974610	-4.05352995	1.18405439

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

H	6.98438940	-5.20207023	1.09802401	O	4.61995022	2.02572934	-2.28602044
H	5.31439354	-4.37106436	-1.84285104	C	4.49645304	-0.20258784	-3.34572841
H	2.92209410	-3.43664424	-0.14208951	O	5.28488312	-1.37731614	-3.64616020
H	2.53539487	-3.99250277	-3.05142248	C	3.70918127	0.14578568	-4.61730306
H	3.39796845	-2.46797619	-2.65048206	O	2.67175561	-0.77894470	-4.89001933
H	1.54168029	-1.64019578	-2.03131800	C	4.46541188	3.22809503	-3.03129848
C	3.20911584	-0.20092572	3.07978026	C	5.00032545	4.41290949	-2.18479499
C	3.22227616	-0.40891298	1.54528679	O	6.34213888	4.21134462	-1.81856867
H	3.87947025	-1.26573252	1.28833722	C	4.04884411	4.70253485	-1.00234313
C	2.28404182	1.02960629	3.37938409	O	4.43356304	5.91232406	-0.38318671
H	2.26663363	1.22762382	4.46654977	C	2.58045729	4.78152990	-1.48726212
C	1.78318604	-0.67363123	1.03423676	O	1.74495906	4.87390573	-0.31134582
H	1.82192493	-0.82609433	-0.05763793	C	2.16787586	3.56243325	-2.34762326
C	0.85385698	0.75864404	2.88265411	O	3.12194854	3.42151438	-3.42073031
H	0.22659741	1.63793925	3.13246449	C	0.75629521	3.64053167	-2.99807764
C	0.87283636	0.53046066	1.35809337	O	-0.09331895	2.55705186	-2.63439170
H	-0.15591343	0.32886200	0.99214322	C	1.04976900	6.05761450	-0.03770436
C	1.20664477	-1.92759980	1.71885804	C	1.14928253	6.42419054	1.46456013
H	0.18513400	-2.12809189	1.33880498	O	2.51425491	6.47704905	1.84966830
H	1.83014913	-2.81181244	1.48152850	C	0.35696255	5.43982308	2.33682450
C	0.30153357	-0.49476573	3.58677172	O	0.37747642	5.92642783	3.67420923
H	0.27689142	-0.33507427	4.68398817	C	-1.07794971	5.23681192	1.81217518
H	-0.73893905	-0.67416882	3.26122758	O	-1.63295988	4.15734991	2.59134423
C	2.61754098	-1.46496835	3.75232132	C	-1.01800291	4.89408506	0.30616291
H	3.26653318	-2.33649026	3.52571098	O	-0.32715422	5.95378096	-0.38062617
H	2.60951616	-1.34646315	4.84982624	C	-2.35610632	4.65650138	-0.42047250
C	1.18318552	-1.71561253	3.24611740	O	-2.34328292	3.40816944	-1.10988629
H	0.77636899	-2.61820865	3.74079834	C	-2.91073015	4.24543737	3.16218729
C	4.56599656	0.15101562	3.71481302	C	-2.86940968	3.71114985	4.62018950
C	5.95134269	2.18744487	4.02276529	O	-1.81745013	4.28958930	5.40548128
H	6.73682423	1.66438768	4.60166290	C	-2.67749796	2.18710493	4.66062054
H	6.40766769	2.95698779	3.37550484	O	-2.84311573	1.68911503	5.98564254
C	4.90048213	2.85340982	4.95577617	C	-3.67410713	1.45301534	3.74385698
C	3.30996979	2.09323117	6.70689432	O	-3.26838984	0.08446854	3.72420952
C	2.68832323	3.30113238	7.08335390	C	-3.64296447	2.10158211	2.33279322
C	2.64793055	0.86245229	6.92752416	O	-3.89255693	3.51820798	2.44823270
C	1.41038831	3.26547787	7.67848385	C	-4.65644777	1.54565404	1.32781916
H	3.18219882	4.25930409	6.90652587	O	-4.37762740	2.02220238	0.01304220
C	1.35286326	0.83513848	7.47843960	C	-4.21597335	-0.97237456	3.85850584
H	3.12002788	-0.07468257	6.60961371	C	-3.75419974	-1.91364774	4.99504475
C	0.74285319	2.04496365	7.86670223	O	-3.51730430	-1.24765240	6.22113589
H	-0.25040309	2.06277437	8.32370453	C	-2.52699144	-2.74234431	4.56084273
O	4.95025239	-0.36827558	4.76957211	O	-2.21091113	-3.71345171	5.55434168
O	4.34340636	3.91209987	4.68385888	C	-2.75677133	-3.45586942	3.21895913
C	0.70652044	4.50840278	8.13272096	O	-1.52436415	-4.06661339	2.83089689
C	0.60537942	-0.46476690	7.53985781	C	-3.21197874	-2.39582961	2.18038065
O	1.50986915	5.58879910	8.14563751	O	-4.37934333	-1.69497089	2.66670542
H	0.94304580	6.36712811	8.34044454	C	-3.55341225	-2.92901421	0.79252983
O	-0.61738725	-0.32947551	8.09074756	O	-3.49133264	-1.83087524	-0.11065508
H	-1.20290556	-1.14842799	7.92600386	C	-1.44191023	-5.47632918	2.61156294
O	1.01775458	-1.53241558	7.10412849	C	-0.24622006	-6.03865678	3.41341800
O	-0.46104818	4.53881281	8.49103839	O	-0.30078033	-5.78645569	4.80459473
N	5.23469753	1.22729003	3.16935056	C	1.07547470	-5.53047959	2.80744529
H	4.90739812	1.59437296	2.27581822	O	2.19412511	-6.10170228	3.47767249
N	4.55988122	2.05888893	6.04088017	C	1.16331630	-5.87318913	1.31704086
H	4.98957143	1.12604418	6.01029094	O	2.33747786	-5.21678127	0.81402150
H	1.22690398	1.43440979	0.82975538	C	-0.10624763	-5.39096939	0.56299624
H	2.68227007	1.93903971	2.88795536	O	-1.31444165	-5.80565057	1.25258275
H	3.63077818	0.48537462	1.03452238	C	-0.22769353	-5.90286675	-0.89813220
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C	5.97602142	-1.95075133	-2.56734392	O	-0.58152621	-4.89204963	-1.81647502
C	6.95009504	-0.91968788	-1.95676895	C	3.25942513	-5.89919135	-0.01831434
O	7.67680783	-1.41135123	-0.84463205	C	4.68963026	-5.57976306	0.47385654
C	6.21159155	0.38876459	-1.60209809	O	4.87987873	-5.84356974	1.85235762
O	7.14112223	1.37971905	-1.17739874	C	5.08164832	-4.12851260	0.12355150
C	5.39921090	0.93143719	-2.78767816	O	6.44906151	-3.88797154	0.44101953
				C	4.84804712	-3.81109083	-1.36252617
				O	5.11012042	-2.41524191	-1.53642276
				C	3.37863371	-4.17121207	-1.71350133

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O	3.12346639	-5.55416989	-1.37707057	H	5.54782880	-4.41113249	-1.98346492
C	2.95516747	-3.98982197	-3.17889900	H	2.72777798	-3.51875030	-1.09866663
O	1.54480866	-3.80082868	-3.30256573	H	3.21291009	-4.90836835	-3.74142857
H	6.53926763	-2.80530046	-2.99394393	H	3.48744244	-3.13523412	-3.63798412
H	7.69902974	-0.67992801	-2.73856762	H	1.36022150	-2.85802383	-3.07368509
H	7.11166245	-2.04850208	-0.34585523	C	0.93346144	-0.43184899	0.07057960
H	5.49516475	0.16454048	-0.78153723	C	2.43450576	-0.03798472	-0.00154961
H	7.73461148	0.93710161	-0.53486126	H	2.57570882	0.78247806	-0.72888484
H	6.09976147	1.29171203	-3.57178305	C	0.80634562	-1.60634033	1.09130978
H	3.76404493	-0.45290351	-2.55658656	H	-0.24775344	-1.93325043	1.17968589
H	4.39544355	0.11817190	-5.48759186	C	2.96614339	0.39223118	1.38594620
H	3.31073633	1.17851368	-4.51864781	H	4.03465034	0.67315376	1.28501473
H	2.05622911	-0.75927719	-4.12750928	C	1.33531143	-1.17648957	2.48344727
H	5.03849220	3.16450597	-3.97656163	H	1.21748518	-2.02932749	3.18375605
H	4.99522434	5.31175087	-2.83514424	C	2.82591172	-0.78314480	2.37920848
H	6.43709720	3.31855296	-1.41321681	H	3.21765075	-0.49671022	3.37882822
H	4.11948215	3.84740076	-0.28931179	C	2.15777209	1.60531757	1.89499767
H	3.91509463	6.00790466	0.44627996	H	2.53677102	1.93345680	2.88663332
H	2.46614847	5.70581689	-2.09210212	H	2.27831333	2.46443790	1.20510745
H	2.19096929	2.65375205	-1.71626633	C	0.52312339	0.03326192	2.99765271
H	0.91680562	3.61092001	-4.09534131	H	-0.54595989	-0.23872284	3.11391786
H	0.27601374	4.61166460	-2.75704949	H	0.88763894	0.33576103	4.00334968
H	-0.81622613	2.88272664	-2.04624272	C	0.12723102	0.78260575	0.61567363
H	1.43894597	6.89389918	-0.65031898	H	0.19289628	1.61894147	-0.10716862
H	0.68083151	7.42964954	1.57262996	H	-0.94952629	0.52657184	0.70969402
H	2.53587286	6.56878061	2.82367526	C	0.66860253	1.20829954	2.00381353
H	0.87089582	4.45622202	2.27986505	H	0.07712654	2.07455349	2.36215191
H	-0.06083797	5.24607516	4.23026954	C	0.44451794	-0.88982607	-1.33360757
H	-1.67160274	6.16149645	1.97837146	C	-1.44341705	-1.59848908	-2.75868668
H	-0.43174861	3.96143419	0.21234185	H	-0.74437882	-1.35886843	-3.58073517
H	-2.49052866	5.47081458	-1.15954231	H	-1.52295944	-2.69965691	-2.67079954
H	-3.21288749	4.68418977	0.27898694	C	-2.85798154	-1.08884908	-3.09611647
H	-2.92347068	2.76434936	-0.61639645	C	-4.20044565	0.81671188	-3.87561017
H	-3.26915410	5.29641359	3.14996725	C	-5.06841186	0.23317836	-4.82019599
H	-3.85461352	3.94034309	5.07982373	C	-4.59503387	1.98195353	-3.20113515
H	-2.12214918	5.14884490	5.75470047	C	-6.32084337	0.82180711	-5.08970686
H	-1.65402847	1.95876512	4.29362701	H	-4.76825493	-0.67722978	-5.34763741
H	-2.20170941	2.16543022	6.55060753	C	-5.86153102	2.55431812	-3.44326313
H	-4.69456145	1.54261152	4.17658219	H	-3.91910262	2.45059760	-2.48069389
H	-2.63048339	1.94179964	1.91141184	C	-6.71792795	1.98436901	-4.40287577
H	-4.58411241	0.44229959	1.30705598	H	-7.70365548	2.41430197	-4.61106929
H	-5.68408663	1.82976311	1.63750301	O	1.25032524	-1.15180238	-2.24633627
H	-5.02072995	2.70927885	-0.28436568	O	-3.84471123	-1.81206076	-2.96269639
H	-5.21424536	-0.55188409	4.09394389	C	-7.27710342	0.25083014	-6.09647905
H	-4.58511201	-2.62294780	5.18421104	C	-6.30548139	3.69263985	-2.58448890
H	-3.09572671	-0.37351058	6.03817910	O	-6.78220948	-0.84872756	-6.72402432
H	-1.66671227	-2.04876071	4.42629228	H	-7.47634598	-1.14273405	-7.35470411
H	-2.22460315	-3.24207727	6.41442103	O	-7.27431619	4.44482671	-3.15006291
H	-3.54638768	-4.22785892	3.34335758	H	-7.52870365	5.12560994	-2.48703004
H	-2.38436685	-1.66973707	2.05989459	O	-5.88261363	3.94054764	-1.46002390
H	-4.57462041	-3.37050688	0.82041524	O	-8.37628616	0.70651418	-6.34314380
H	-2.83594821	-3.72857557	0.51194413	N	-0.89913395	-1.02159099	-1.52828227
H	-3.83105759	-2.10138571	-0.99532816	H	-1.54507552	-1.01595057	-0.73146194
H	-2.38417108	-5.95696014	2.94363231	N	-2.94620017	0.20526528	-3.57024168
H	-0.27263754	-7.14195780	3.29350020	H	-2.12264589	0.80970739	-3.48929617
H	-0.79209199	-4.94656658	4.97885486	H	3.42842791	-1.64989321	2.03410695
H	1.09776546	-4.42265094	2.90789671	H	1.38322307	-2.47901457	0.72821475
H	1.99347428	-6.03296913	4.43550974	H	3.02287180	-0.89481491	-0.37657457
H	1.27779806	-6.97406535	1.21279957				
H	-0.07374338	-4.28673104	0.52592466				
H	-1.02116785	-6.68074372	-0.89303453				
H	0.71795738	-6.39274261	-1.20478432				
H	0.22138833	-4.62829247	-2.33707888				
H	3.07548325	-6.99134212	0.02975881				
H	5.38091417	-6.25293622	-0.07341335				
H	4.03592426	-5.66321818	2.32991595				
H	4.43037141	-3.44625106	0.71587946				
H	6.58319409	-4.24017515	1.34645993				

7c_gamma-CD_P:

C	1.41077948	-0.43219825	-2.51946778
C	0.52566471	-1.40365224	-1.67581765
H	0.97279846	-2.41515736	-1.69570170
C	0.75104196	0.97699685	-2.49541278
H	1.36807478	1.71136876	-3.05943793
C	0.39516242	-0.89947260	-0.22153006
H	-0.23172597	-1.61719123	0.34878720

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C	0.60633205	1.47532374	-1.03330668	C	6.84781561	-0.92704398	2.44076473
H	0.12036947	2.47107685	-1.04428746	C	7.62005498	-2.04341458	1.70909374
C	-0.27134774	0.49196454	-0.22615158	C	6.68910362	-2.92530257	0.86889231
H	-0.41460691	0.87324444	0.80433156	C	5.49905998	-3.44064807	1.70386554
C	1.79981995	-0.81355331	0.41657167	C	4.83065675	-2.27506881	2.46802880
H	1.73119123	-0.49706531	1.47747491	C	3.78900290	-2.70359692	3.50800955
H	2.27512189	-1.81653482	0.41656101	O	8.63590671	-1.47301040	0.88826823
C	2.00642066	1.57620115	-0.38546361	O	7.49601667	-3.96155177	0.34121143
H	2.64007383	2.30483789	-0.93470904	O	4.53126639	-4.02979205	0.81977980
H	1.91596063	1.95522335	0.65388185	O	5.81746211	-1.51882239	3.20208368
C	2.81739860	-0.32641638	-1.84181812	O	3.12854752	-1.59417864	4.08529050
H	3.30985693	-1.31904700	-1.85803714	C	4.43704974	-5.43009842	0.71447213
H	3.46336018	0.36689104	-2.42430753	C	4.59857164	-5.88822349	-0.75301388
C	2.67129807	0.18005532	-0.38775942	C	3.41150634	-5.43801749	-1.60856220
H	3.68093567	0.24417003	0.06593990	C	2.09731260	-5.92513055	-0.97536211
C	1.60327105	-1.05693193	-3.91869401	C	2.00469410	-5.49062211	0.50497045
C	1.44205168	-0.72948287	-6.38862792	C	0.83545859	-6.12313147	1.27397621
H	1.71709686	-1.80104833	-6.35181006	O	5.82059862	-5.41050443	-1.30446404
H	0.45685308	-0.65662886	-6.88891117	O	3.63500549	-5.95594418	-2.90986316
C	2.44962450	0.01261034	-7.30243435	O	0.99329781	-5.37551724	-1.71053758
C	4.61346586	1.31043462	-7.13394765	O	3.19752596	-5.90860987	1.20843618
C	4.76280510	1.63890742	-8.49993495	O	0.85927201	-7.53965605	1.24442561
C	5.59249645	1.73275283	-6.21232707	C	0.37560858	-6.19187117	-2.67603391
C	5.87894738	2.39214360	-8.91788755	C	0.25456455	-5.42847634	-4.03025349
H	4.01313296	1.30791538	-9.22151659	C	-0.84292477	-4.35104422	-3.97469799
C	6.70437993	2.48469892	-6.63243476	C	-2.16048380	-4.86936633	-3.34936200
H	5.50705216	1.48655942	-5.14534273	C	-1.86026686	-5.59505901	-2.01881581
C	6.84857534	2.82098992	-7.99102880	C	-3.04677378	-6.28155719	-1.33223251
H	7.70307775	3.40853982	-8.34205549	O	1.50533801	-4.92546236	-4.46979469
O	1.99520536	-2.22302591	-4.04916135	O	-1.06297171	-3.74194302	-5.25518904
O	2.27828988	0.03852806	-8.51110235	O	-2.97912893	-3.71837805	-3.13911588
C	6.07815173	2.76739862	-10.35828767	O	-0.89769139	-6.63833780	-2.25891750
C	7.69915470	2.88515114	-5.58394047	O	-2.67104604	-6.82663961	-0.08439892
O	5.06569712	2.34323018	-11.16142675	C	-4.34579024	-3.70833865	-3.52853589
H	5.29625489	2.64192038	-12.06894145	C	-4.55048441	-2.59999274	-4.58188717
O	8.68817270	3.67566869	-6.06616699	C	-4.35483161	-1.22332555	-3.92667559
H	9.27134834	3.89254668	-5.30525938	C	-5.26392212	-1.02187390	-2.70527320
O	7.64513538	2.53844982	-4.41741863	C	-5.11729938	-2.23781349	-1.74141161
O	7.03241155	3.38616608	-10.78664957	C	-6.21241144	-2.35460086	-0.65514420
N	1.36521193	-0.26134287	-5.01256492	O	-3.72057703	-2.73616822	-5.72056538
H	0.97870668	0.66727965	-4.85445917	O	-4.59272615	-0.19457783	-4.88763737
N	3.51556925	0.57812224	-6.62998304	O	-4.82016105	0.17137906	-2.05344324
H	3.50644458	0.45398767	-5.61728953	O	-5.20045812	-3.50062632	-2.43502509
H	-1.28271682	0.42517969	-0.68064947	O	-6.53698850	-1.15597601	0.01492218
H	-0.25242484	0.94557411	-2.97414946	C	-5.73328413	1.21101840	-1.70593296
H	-0.48214151	-1.47889700	-2.13859059	C	-5.80329521	2.31196018	-2.78947644
C	2.56933092	7.01909429	-1.33927467	C	-4.46463047	3.06859878	-2.89993016
C	3.72350495	6.70757191	-2.31831330	C	-4.03438949	3.60294525	-1.52545955
C	4.46896749	5.42460973	-1.88610700	C	-4.02405243	2.42533288	-0.51466392
C	4.85027206	5.51477936	-0.38908265	C	-3.69998542	2.84850921	0.93099425
C	3.67680404	5.91810724	0.53080372	O	-6.23996774	1.88327355	-4.06599322
C	4.09872008	6.28793177	1.96075915	O	-4.63089497	4.13496774	-3.84853691
O	3.25990731	6.70658560	-3.64431124	O	-2.72067113	4.18410416	-1.53838776
O	5.60775621	5.27290577	-2.69415526	O	-5.31315865	1.78332710	-0.49118783
O	5.35270742	4.22715209	0.00619000	O	-2.33227257	3.14725027	1.11108758
O	3.02408591	7.10857686	0.00570766	C	-2.58765613	5.53328556	-2.00594477
O	5.01513744	7.36821786	2.00102916	C	-1.68243691	5.59605424	-3.26449257
C	6.61651543	4.12242149	0.61779829	C	-0.21334998	5.37808129	-2.89147824
C	7.52119122	3.14751640	-0.17217859	C	0.22840622	6.35602502	-1.79826295
C	7.06964220	1.68484294	-0.02700707	C	-0.72252117	6.24152159	-0.57773664
C	6.88623762	1.33131553	1.45859957	C	-0.53296617	7.31079422	0.52803113
C	5.96654235	2.36295661	2.15327701	O	-1.99003145	4.64967172	-4.26765715
C	5.83246945	2.17981349	3.67034393	O	0.61561361	5.53932508	-4.03686254
O	7.56316576	3.56478850	-1.52746686	O	1.57181934	6.02092082	-1.45023713
O	8.03635681	0.88175991	-0.67538686	O	-2.09757264	6.38105155	-1.00089885
O	6.32443865	0.01147521	1.51958991	O	0.54688184	7.07026291	1.39323502
O	6.51073300	3.68461657	1.96408147	H	2.14573867	8.01658464	-1.57172621
O	7.07633198	2.22560043	4.34619064	H	4.44862998	7.54399932	-2.25209202

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H	3.76740624	4.56106434	-1.99984865		H	-3.59231211	5.93048234	-2.24408533
H	5.65067900	6.27492661	-0.28813840		H	-1.78409196	6.63596334	-3.65824588
H	2.94067626	5.08919670	0.57228293		H	-0.11119487	4.34461217	-2.49188325
H	4.60795728	5.42347079	2.42341512		H	0.18753827	7.39027161	-2.20358394
H	3.17937331	6.50251272	2.55341471		H	-0.55923737	5.25074578	-0.10303260
H	2.49166934	6.09465138	-3.72106505		H	-1.45284209	7.28103768	1.14396305
H	6.17330249	4.55454763	-2.31565834		H	-0.49146040	8.32242096	0.05400534
H	4.58472797	8.11985896	1.54732388		H	-2.97663135	4.56287845	-4.34211234
H	7.09692644	5.11791656	0.68015614		H	0.17200881	5.06181896	-4.76798666
H	8.53854742	3.21867180	0.27549530		H	1.39855867	7.22119642	0.92184655
H	6.07642894	1.57594718	-0.52345320					
H	7.87625827	1.34409449	1.95692398					
H	4.95415240	2.30346156	1.70038199					
H	5.38723958	1.18981629	3.88156673					
H	5.12873452	2.95681137	4.05107387					
H	7.91460186	2.83728240	-2.08295643					
H	8.10324754	0.00934516	-0.21532213					
H	7.48758697	3.08349610	4.11773237					
H	7.50085169	-0.41984389	3.17652273					
H	8.08944220	-2.68080840	2.49147496					
H	6.26561891	-2.29813673	0.05236477					
H	5.86666310	-4.20220132	2.42459834					
H	4.33943877	-1.60932713	1.73244240					
H	3.01373768	-3.32075948	3.01853907					
H	4.29192608	-3.33435066	4.28078817					
H	8.96751337	-2.21391904	0.33582605					
H	6.97964238	-4.44124495	-0.35552866					
H	3.82443924	-1.02096539	4.46392868					
H	5.20348961	-5.91634688	1.34969761					
H	4.60974176	-7.00125454	-0.74035562					
H	3.39192488	-4.32536967	-1.62833057					
H	2.05461876	-7.03194010	-1.01093787					
H	1.90864174	-4.38517669	0.55393010					
H	-0.12632865	-5.81694265	0.82548766					
H	0.86230096	-5.73335768	2.31814522					
H	5.72461334	-5.48678716	-2.27861896					
H	2.97191495	-5.55743359	-3.53395169					
H	1.71209169	-7.81777773	1.63442476					
H	0.96536229	-7.11407232	-2.83572776					
H	-0.05811046	-6.19968126	-4.77039681					
H	-0.49598892	-3.52488685	-3.32951223					
H	-2.65543129	-5.57363500	-4.05490307					
H	-1.43690909	-4.85320857	-1.31109675					
H	-3.46238182	-7.05860298	-2.01972174					
H	-3.84278804	-5.54044567	-1.13334026					
H	1.58685970	-3.95316742	-4.28572099					
H	-1.07946120	-4.44127667	-5.94053425					
H	-1.90950654	-7.42151479	-0.24233611					
H	-4.63067078	-4.69575925	-3.94391778					
H	-5.59259971	-2.67264584	-4.95304858					
H	-3.30411530	-1.15371047	-3.56786658					
H	-6.31712805	-0.92216280	-3.04005573					
H	-4.11773857	-2.14543682	-1.26340087					
H	-5.90478872	-3.16117076	0.05074739					
H	-7.14510538	-2.69090000	-1.14857932					
H	-2.79059343	-2.91289628	-5.42188441					
H	-4.22056080	-0.51898867	-5.73653884					
H	-5.73108914	-0.74853329	0.38824199					
H	-6.73423637	0.78672897	-1.50921859					
H	-6.57209880	3.03341132	-2.44578799					
H	-3.67991108	2.37159009	-3.26443218					
H	-4.77241787	4.36184489	-1.18393913					
H	-3.25448215	1.69420270	-0.83313233					
H	-3.93845039	1.99592185	1.59606743					
H	-4.36289887	3.69692501	1.22761563					
H	-5.62926924	1.17884863	-4.40880659					
H	-5.23324944	3.76728425	-4.53700586					
H	-2.08916460	3.77552701	0.40095368					

7c_gamma-CD_S:

6	-0.006100673	-0.924325040	0.267722142
6	1.171378683	-1.837344504	-0.199519842
1	0.763104645	-2.768882585	-0.637262141
6	0.592749857	0.373522444	0.883657160
1	-0.216843956	1.054500511	1.218401490
6	2.051215511	-1.097806032	-1.237743299
1	2.880603417	-1.770823871	-1.543844937
6	1.470205213	1.109112719	-0.160526310
1	1.880371123	2.029419859	0.304804714
6	2.630796645	0.191049799	-0.608555429
1	3.272117263	0.719208816	-1.345085899
6	1.199846387	-0.721137487	-2.473103460
1	1.831111114	-0.208894698	-3.230113232
1	0.796052485	-1.636359456	-2.958892196
6	0.605358389	1.488333392	-1.384376976
1	-0.225976767	2.152364594	-1.072078022
1	1.213009782	2.054417986	-2.121446852
6	-0.836464983	-0.549770579	-0.998812167
1	-1.234812091	-1.477957628	-1.452427657
1	-1.708124977	0.068054475	-0.707920010
6	0.039586369	0.200323789	-2.027622191
1	-0.587448321	0.466189577	-2.905600808
6	-0.922717013	-1.734791742	1.220303782
6	-1.762126488	-2.004554085	3.565945354
1	-2.193647198	-2.916350949	3.112846167
1	-1.042009356	-2.297896143	4.353146303
6	-2.861773518	-1.17331781	4.293265875
6	-5.170543597	-0.244879391	3.878417381
6	-5.477466063	0.220056105	5.178334478
6	-6.121258791	-0.068175445	2.850009357
6	-6.727214811	0.831659325	5.424092256
1	-4.747316296	0.101388165	5.981815119
6	-7.364728053	0.535211944	3.098446831
1	-5.887169631	-0.387321170	1.830874566
6	-7.673933844	0.988697346	4.394301566
1	-8.636123802	1.459528242	4.618392504
8	-1.526726736	-2.744963757	0.812006423
8	-2.719242092	-0.834463155	5.460615202
6	-7.111110744	1.335942166	6.785080153
6	-8.314658472	0.656266066	1.947723126
8	-6.131293119	1.159227054	7.712310143
1	-6.486644817	1.523352040	8.553168908
8	-9.444203873	1.341947232	2.265907526
1	-9.995570561	1.350792377	1.452641180
8	-8.133984140	0.199582771	0.831445818
8	-8.177397185	1.852351008	7.059695284
7	-1.051658358	-1.293195233	2.505268895
1	-0.476391919	-0.507204926	2.801520925
7	-3.974241687	-0.902698217	3.520460284
1	-3.983391309	-1.262282492	2.553104915
1	3.280900605	-0.057200531	0.254501765
1	1.220826942	0.117310912	1.764240631
1	1.787182941	-2.129866957	0.674323880
6	2.492518629	7.109071766	-1.090079214
6	3.647015992	6.799742782	-2.070029609

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

1	-4.549061309	-4.831173522	-3.823577812	H	5.49352985	0.48925535	1.05657710
1	-5.461618686	-2.845451628	-4.848077793	H	5.23630025	-1.26219426	0.93196714
1	-3.144683698	-1.176019599	-3.727053061	C	6.23941188	-0.38493360	-0.80510387
1	-6.044200386	-1.212612349	-2.711415248	C	8.72804234	-0.79762091	-1.04226564
1	-3.398747056	-2.289930289	-1.542712397	C	8.83588876	-0.69070841	-2.44641660
1	-5.390501597	-3.414529714	-0.000155128	C	9.87760491	-1.08182592	-0.27763317
1	-5.973441128	-1.727240557	-0.107759485	C	10.09401617	-0.87193638	-3.05805100
1	-2.684706476	-3.060477400	-5.357930563	H	7.95084556	-0.47160631	-3.04786941
1	-4.310923297	-0.572330532	-5.710846533	C	11.12753103	-1.26050749	-0.89453005
1	-3.294124459	-2.420357998	0.696650693	H	9.82573512	-1.17236059	0.81669464
1	-6.491811529	0.531600733	-1.360467219	C	11.24074356	-1.15590346	-2.29214782
1	-6.517249582	2.836973462	-2.151107089	H	12.20357931	-1.29154261	-2.79557444
1	-3.612438365	2.430712875	-3.090187168	O	2.96521372	-0.51366377	1.82958177
1	-4.761138210	4.223706351	-0.865423289	O	5.92583884	-0.22523116	-1.97691279
1	-3.073712462	1.640420050	-0.728042943	C	10.26900266	-0.77410295	-4.54650850
1	-3.699167478	1.739442999	1.735648406	C	12.29350375	-1.56296930	-0.00058693
1	-4.207653373	3.441910441	1.493756411	O	9.10429521	-0.49861550	-5.19391289
1	-5.556774582	1.110082336	-4.214472468	H	9.32401934	-0.45531730	-6.15073947
1	-5.285314877	3.777323143	-4.238259540	O	13.45407738	-1.71431961	-0.69049582
1	-1.972522616	3.670604829	0.593371281	H	14.14986769	-1.90968654	-0.02452055
1	-3.686391139	5.913785447	-1.888965248	O	12.22597582	-1.66585873	1.20927960
1	-1.942568389	6.772618632	-3.309923310	O	11.32540805	-0.92271568	-5.12790616
1	-0.151103812	4.482301546	-2.327272306	N	3.88331018	-0.10374058	-0.17871219
1	0.081366389	7.511277553	-1.867448705	H	3.81425513	0.09226871	-1.17795325
1	-0.586482039	5.270275887	0.151226988	N	7.51198458	-0.63941921	-0.33906337
1	-1.516024216	7.233948912	1.483963790	H	7.59786314	-0.74397632	0.67210287
1	-0.603163515	8.336065390	0.411719448	C	-4.65850169	-3.64706093	-3.48081825
1	-3.084181530	4.692319555	-4.062186326	C	-4.10192259	-3.29762101	-4.87430954
1	0.096810115	5.296887242	-4.542748913	O	-3.09543901	-4.19827831	-5.29816410
1	1.329984265	7.262464518	1.206261201	C	-3.59813772	-1.84429749	-4.89899495
				O	-3.24018917	-1.45847676	-6.21849553
				C	-4.66487176	-0.88183745	-4.37218387
				O	-4.07638696	0.41823546	-4.37638402
				C	-5.11029747	-1.33396261	-2.95704170
				O	-5.60241937	-2.69093818	-3.05552425
				C	-6.23785332	-0.49655191	-2.31860537
				O	-6.09742490	-0.33462307	-0.90822448
				C	-4.83671314	1.52016561	-4.83282718
				C	-3.90920754	2.43167517	-5.67140454
				O	-3.26342904	1.69521695	-6.67989221
				C	-2.94384305	3.23659134	-4.76743538
				O	-2.38340056	4.28107789	-5.54437951
				C	-3.66171925	3.80751291	-3.52555604
				O	-2.63253501	4.38702475	-2.69761281
				C	-4.45092676	2.70278553	-2.80452397
				O	-5.42212693	2.21843856	-3.75486207
				C	-5.20054165	3.08738850	-1.52025830
				O	-5.01898538	2.09209485	-0.51649337
				C	-2.80927387	5.69764182	-2.20372348
				C	-1.41448248	6.37153450	-2.14680716
				O	-0.66430738	6.16390265	-3.34516642
				C	-0.58858605	5.92290924	-0.92996116
				O	0.54166506	6.76259712	-0.74823370
				C	-1.41061182	5.90379233	0.36177318
				O	-0.57254888	5.32799072	1.35173047
				C	-2.68495578	5.06789995	0.10753334
				O	-3.43254517	5.73348061	-0.93873264
				C	-3.61304034	4.84549036	1.32104470
				O	-3.93771899	3.46896669	1.47173280
				C	-0.48203591	5.89481904	2.65108727
				C	1.01035510	5.82512958	3.05579597
				O	1.80463352	6.52335217	2.12624010
				C	1.41490699	4.35161654	3.25998569
				O	2.69428038	4.28180102	3.85316147
				C	0.37984314	3.62811627	4.14416496
				O	0.73504016	2.23883368	4.14063618
				C	-1.06567860	3.81147908	3.65700660
				O	-1.32784704	5.22768927	3.55940929

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C	-2.13292181	3.18868003	4.57480703	H	1.39907727	3.86146715	2.25949867
O	-3.16646410	2.53808549	3.84015216	H	2.90291407	3.32977420	3.99894023
C	1.05663531	1.62770212	5.36429814	H	0.46265950	4.04188674	5.17197512
C	2.25135400	0.65579711	5.13006000	H	-1.16247683	3.34677621	2.65774670
O	3.26991965	1.27610299	4.34495816	H	-1.65030166	2.46756659	5.26191898
C	1.79027180	-0.66510260	4.49731082	H	-2.57090450	4.00678117	5.18571307
O	2.82665983	-1.64258663	4.49767154	H	-3.12654457	1.55033779	4.01567801
C	0.52656486	-1.22682748	5.14791733	H	1.34263699	2.39058413	6.11461708
O	0.18310500	-2.35859145	4.36388825	H	2.69740580	0.43050766	6.11896183
C	-0.54280753	-0.11592705	5.08359524	H	3.11020251	1.03060327	3.40825077
O	-0.06377185	0.95847886	5.92013985	H	1.50166290	-0.44954379	3.45300407
C	-1.98887645	-0.48756912	5.47699107	H	3.32926809	-1.49111672	3.67104179
O	-2.92549873	-0.06382228	4.48966566	H	0.70879860	-1.51609092	6.20498714
C	-0.29430470	-3.53552621	4.97319155	H	-0.59699807	0.23324924	4.03317535
C	0.50264529	-4.71145371	4.37059129	H	-2.22269334	0.01892289	6.43636814
O	1.90001042	-4.54090261	4.50784642	H	-2.07942733	-1.58028108	5.62709133
C	0.11183086	-4.90296731	2.89442564	H	-3.25787502	-0.83810613	3.94513979
O	0.69475568	-6.08415583	2.35724294	H	-0.16010621	-3.49703033	6.07323816
C	-1.40914130	-4.97176437	2.72005567	H	0.22832168	-5.63461267	4.92025716
O	-1.64195219	-5.06455623	1.31480983	H	2.10930152	-3.58379828	4.35805924
C	-2.03216552	-3.69860109	3.34835961	H	0.47078567	-4.00701324	2.34107831
O	-1.67719883	-3.68927725	4.74866363	H	1.63157754	-6.06971264	2.64518846
C	-3.55711504	-3.52225140	3.26605676	H	-1.80331517	-5.87292690	3.23637796
O	-3.91828528	-2.16042780	3.04798753	H	-1.58059175	-2.82044136	2.84502636
C	-2.57683041	-5.99672183	0.81777553	H	-3.98818685	-3.86067615	4.23128415
C	-2.03162632	-6.49769260	-0.53813407	H	-3.96626816	-4.16668083	2.46819618
O	-0.71077212	-6.99640335	-0.43786026	H	-4.23373524	-2.04692750	2.10159135
C	-2.13017323	-5.38968735	-1.60946936	H	-2.69986836	-6.84326407	1.52312013
O	-1.82562393	-5.89974554	-2.90076227	H	-2.67613989	-7.33704716	-0.87027259
C	-3.53627740	-4.77829883	-1.62481144	H	-0.24275101	-6.47320033	0.25408443
O	-3.55452503	-3.74341400	-2.60260826	H	-1.40956184	-4.59082912	-1.32841531
C	-3.83834210	-4.26619651	-0.20015158	H	-0.99368342	-6.40779493	-2.80203496
O	-3.85911294	-5.42471696	0.66428079	H	-4.27306505	-5.56663988	-1.88834669
C	-5.12062636	-3.44566120	0.01364284	H	-3.00663573	-3.60416699	0.10617634
O	-4.75746976	-2.14464759	0.47103968	H	-5.74745014	-3.97375890	0.76606411
H	-5.20596439	-4.61057523	-3.51768162	H	-5.70110870	-3.36547497	-0.92435887
H	-4.93497350	-3.37500202	-5.60197781	H	-5.31041911	-1.44699203	-0.00835474
H	-2.57115742	-4.46187713	-4.50605622				
H	-2.72249379	-1.77676108	-4.21741173				
H	-2.68302875	-2.18467483	-6.56815996				
H	-5.54310960	-0.90811024	-5.05262481				
H	-4.22894856	-1.30453589	-2.28433637				
H	-7.19320283	-1.02447388	-2.51829004				
H	-6.28268312	0.49658451	-2.79986283				
H	-5.70301760	0.56974164	-0.71344648				
H	-5.67950419	1.17292737	-5.46375085				
H	-4.55472983	3.18175126	-6.17242859				
H	-3.04683828	0.80641741	-6.31740925				
H	-2.15847019	2.53347912	-4.39698593				
H	-1.94829154	4.90872978	-4.93237613				
H	-4.36687014	4.59917426	-3.85523834				
H	-3.74763548	1.88902527	-2.53952800				
H	-6.27845709	3.18928985	-1.77248094				
H	-4.84549431	4.06665972	-1.15464679				
H	-4.65365765	2.52701975	0.31376283				
H	-3.47776857	6.27260973	-2.87619821				
H	-1.57076872	7.46349657	-2.06817127				
H	-0.51846170	5.19602425	-3.40286275				
H	-0.26862701	4.87008596	-1.10922886				
H	0.98138151	6.83744063	-1.61953645				
H	-1.69613299	6.94086292	0.63981987				
H	-2.37782027	4.06590027	-0.24734870				
H	-4.53677874	5.44025209	1.15213607				
H	-3.12722431	5.21615057	2.24293043				
H	-3.65285681	3.11227400	2.37183092				
H	-0.81786320	6.95111642	2.63496259				
H	1.12217601	6.34102095	4.03029990				
H	1.48188945	6.30067387	1.22479949				

8c_beta-CD_S:

C	0.21005560	0.33355970	0.04250688
C	-0.00650515	0.11838468	1.57937617
H	0.98636451	0.03929061	2.06214541
C	-1.19269809	0.40677822	-0.61780060
H	-1.06430106	0.58562161	-1.70428882
C	-2.00079858	-0.88044808	-0.35868064
H	-1.49779818	-1.76591726	-0.78538057
H	-2.97045810	-0.79655737	-0.87768163
C	-0.81429549	-1.16979259	1.83176786
H	-0.94871722	-1.31649126	2.92268869
H	-0.25478326	-2.04957709	1.45973161
C	-2.19759443	-1.07882512	1.15615618
H	-2.76522325	-2.01346399	1.32262579
C	-2.97082429	0.11920008	1.74281809
H	-3.97311162	0.19643214	1.26842250
H	-3.13129661	-0.02292291	2.83315703
C	-0.77064775	1.34096609	2.15881217
H	-0.89636954	1.18553454	3.25117338
C	-1.96608237	1.62548009	-0.02975410
H	-2.96561985	1.66977781	-0.51055654
C	-2.17167453	1.41353764	1.49294602
H	-2.72451870	2.28420756	1.90515546
C	0.00265667	2.65344268	1.91239147
H	-0.55139960	3.50691216	2.35737536
H	0.99705459	2.60566695	2.40403621
C	-1.20102104	2.93421573	-0.29490347
H	-1.06975064	3.07536347	-1.38873132
H	-1.77798216	3.80041188	0.09372940

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C	0.97535613	1.67165865	-0.17474010	O	3.88369442	0.36511379	5.82537694
H	1.94838569	1.58366956	0.34238856	C	4.38556657	1.19851415	3.54297560
H	1.18293127	1.82452659	-1.25095297	O	4.77109652	2.48227182	3.97405149
C	0.17908287	2.85907146	0.39302982	C	5.12971463	0.80863392	2.24401644
H	0.73912387	3.79982141	0.19949242	O	4.67008612	1.72527763	1.23844226
C	1.16669344	-0.74341262	-0.51292682	C	4.81245615	-0.64875552	1.86586087
C	1.93701979	-2.26690190	-2.24278025	O	5.25098105	-1.48577380	2.96035869
H	2.80320294	-1.69640683	-2.62689258	C	5.43913840	-1.18215014	0.57029487
H	2.29322186	-2.89499103	-1.40892796	O	4.60219786	-2.14160988	-0.08480600
C	1.37197386	-3.14991052	-3.36091634	C	5.58918258	2.47687188	0.48930967
C	0.41471578	-5.44721915	-3.63221711	C	5.05216050	3.92037974	0.36996068
C	-0.15792285	-5.32389949	-4.91433687	O	4.83058326	4.44883139	1.66773136
C	0.33352333	-6.67752424	-2.95356385	C	3.76692891	3.92708057	-0.46606419
C	-0.84677506	-6.42132318	-5.47162905	O	3.32533171	5.29014238	-0.60253034
H	-0.08551172	-4.37781221	-5.45434482	C	4.01933936	3.25011884	-1.82234151
C	-0.35923681	-7.76465369	-3.50680482	O	2.79482661	3.26882947	-2.55268791
H	0.79346833	-6.79409229	-1.96606149	C	4.56587992	1.82526934	-1.56595765
C	-0.95588320	-7.64091431	-4.77469919	O	5.78894804	1.94755983	-0.80929093
H	-1.50705255	-8.47261526	-5.22622956	C	4.83530106	0.98277020	-2.82461560
O	2.20656745	-0.98570444	0.12660593	O	3.73238099	0.13029658	-3.02108134
O	1.30063440	-2.77512011	-4.54046322	C	2.82107308	3.48497795	-3.96261206
C	-1.51821051	-6.32808275	-6.80761184	C	1.77485775	4.57637881	-4.26850400
C	-0.46025906	-9.00229365	-2.67027436	O	2.05765735	5.75209827	-3.54168037
O	-1.42170672	-5.08300186	-7.35906520	C	0.35680771	4.02509505	-4.02441302
H	-1.87880501	-5.13564929	-8.22716011	O	-0.57503637	4.95425841	-4.54870411
O	-1.07938995	-10.02615183	-3.31740563	C	0.17033953	2.64115650	-4.67835572
H	-1.10353819	-10.77743969	-2.68452499	O	-1.06380891	2.08955260	-4.15739585
O	-0.05193346	-9.10213867	-1.52759672	C	1.33720290	1.65960195	-4.44859124
O	-2.10333241	-7.23936452	-7.35974937	O	2.58903935	2.31720570	-4.69992914
N	0.93715846	-1.33424074	-1.71003348	C	1.27585065	0.47529881	-5.42457954
H	0.03789192	-1.27442613	-2.19433653	O	2.36357524	-0.41079928	-5.24827151
N	0.99957798	-4.38411332	-2.92054929	C	-2.09645645	1.73957732	-5.05372014
H	1.04873774	-4.53254114	-1.88872457	C	-3.43663237	2.26650738	-4.46232763
C	-5.54922576	-1.74316749	-2.81771734	O	-3.31332779	3.59707792	-3.95201292
C	-6.30328881	-1.73231579	-1.47130925	C	-4.00181508	1.34975503	-3.36751764
O	-6.71671994	-0.43168896	-1.08803247	O	-5.33317222	1.70605388	-3.02325249
C	-5.44028032	-2.37420348	-0.36733227	C	-3.95658462	-0.12238297	-3.77709852
O	-6.19222162	-2.58031013	0.82381200	O	-4.43972838	-0.87128274	-2.66865829
C	-4.84124531	-3.71295577	-0.80085631	C	-2.48395698	-0.43895772	-4.14160935
O	-3.82474444	-4.02868171	0.15692177	O	-2.16173059	0.35004174	-5.30543766
C	-4.20441117	-3.58270076	-2.19636422	C	-2.13223299	-1.91632098	-4.38893130
O	-5.14873635	-3.05280224	-3.14783686	O	-1.43195675	-2.37601294	-3.23786748
C	-3.61225317	-4.87775950	-2.78235641	H	-6.20914717	-1.39882253	-3.63922911
O	-2.22659466	-4.99386121	-2.49377526	H	-7.21642791	-2.34869633	-1.59664761
C	-3.58743600	-5.37108642	0.53377004	H	-6.06918755	0.21093398	-1.45664297
C	-3.95625501	-5.51993966	2.02847451	H	-4.59671529	-1.68461961	-0.17319405
O	-5.30471403	-5.16441228	2.21599817	H	-6.61172134	-1.72329457	1.04232454
C	-2.96296698	-4.72887614	2.89786888	H	-5.64000654	-4.48516539	-0.79319031
O	-3.16459906	-5.07567717	4.25610714	H	-3.36792293	-2.87078251	-2.09112529
C	-1.51583614	-5.04010952	2.47702835	H	-3.70733875	-4.82314353	-3.88384027
O	-0.65668423	-4.10900824	3.15248829	H	-4.17352821	-5.77726324	-2.44649613
C	-1.24068689	-4.95022059	0.96547337	H	-2.10677515	-5.26329331	-1.54764798
O	-2.24072480	-5.71970892	0.24516286	H	-4.20789556	-6.06623961	-0.06365917
C	0.15243478	-5.51571011	0.60165066	H	-3.86711681	-6.58901391	2.30494427
O	0.93798152	-4.57459676	-0.12096051	H	-5.43082674	-4.23354807	1.91974433
C	0.26922472	-4.60088224	4.10055325	H	-3.14341399	-3.64294577	2.72192870
C	0.32052710	-3.58325156	5.26738931	H	-2.53395065	-4.56109703	4.80332189
O	-0.99317812	-3.16854079	5.65987815	H	-1.29824997	-6.07582125	2.81272799
C	1.18625385	-2.35525405	4.95122919	H	-1.29939805	-3.89330282	0.64334545
O	1.43369608	-1.59729757	6.12669445	H	-0.01114263	-6.44320320	0.01075106
C	2.52481192	-2.73006790	4.31142965	H	0.68974600	-5.80027580	1.52717432
O	3.12448534	-1.49945477	3.93100779	H	1.84515146	-4.48623421	0.31305322
C	2.26151237	-3.65672986	3.09687630	H	-0.06776676	-5.58525111	4.48258744
O	1.54181986	-4.82875613	3.55308871	H	0.75760866	-4.09032397	6.14746907
C	3.53499954	-4.15292553	2.39417121	H	-1.375557807	-2.73489596	4.86707648
O	3.37185557	-4.30279564	0.98385418	H	0.65195300	-1.73597952	4.19525930
C	4.51370466	-1.27018174	4.14020489	H	0.56710735	-1.44919702	6.55658790
C	4.66480740	0.17799386	4.66879784	H	3.15383663	-3.26430512	5.05605473

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

H	1.65239541	-3.09793737	2.35916133	O	6.16894045	-3.73962377	-0.35606024
H	3.80088902	-5.13521081	2.83816684	C	2.77913042	-4.61298283	-0.60384839
H	4.35863368	-3.44227859	2.58819005	C	2.20622497	-5.65615761	-1.59694705
H	3.90897108	-3.57392080	0.54678457	C	0.71885378	-5.42399228	-1.84997787
H	4.90934514	-1.98454809	4.89003548	C	-0.02825390	-5.30372439	-0.51873503
H	5.72384513	0.31302969	4.96857446	C	0.63258184	-4.22536127	0.35593868
H	3.01496637	-0.06935876	5.67488799	C	-0.03528563	-4.00626850	1.71632320
H	3.29293006	1.15174117	3.30841729	O	2.92286851	-5.63577181	-2.84202327
H	4.64042707	3.10064138	3.21962631	O	0.25589583	-6.50149246	-2.64475475
H	6.22167946	0.93182161	2.40524779	O	-1.37812019	-4.96588838	-0.81827455
H	3.71549790	-0.72471885	1.76558416	O	2.00777114	-4.61796438	0.56787746
H	5.64916342	-0.33578409	-0.11477608	O	-0.96241607	-2.94047739	1.57878098
H	6.39771174	-1.68293486	0.80792516	C	-2.41179550	-5.86797994	-0.53404656
H	3.72673575	-1.68950653	-0.24259658	C	-3.33637180	-5.92488433	-1.76922249
H	6.58709176	2.48075742	0.97150611	C	-3.97007163	-4.55132163	-1.97396876
H	5.82481106	4.51436624	-0.16816611	C	-4.66917042	-4.10938678	-0.68111239
H	4.35749681	5.29711629	1.54392348	C	-3.67743034	-4.12131180	0.49282567
H	3.01412697	3.34157065	0.08826622	C	-4.27037274	-3.71287054	1.84389220
H	2.36410182	5.31394724	-0.43978952	O	-2.58992847	-6.33319388	-2.91226160
H	4.79367280	3.83177618	-2.36868815	O	-4.86018823	-4.63075604	-3.07946613
H	3.82549615	1.25774672	-0.97121265	O	-5.17215038	-2.79276511	-0.89007655
H	5.76832043	0.40262238	-2.63714869	O	-3.15895105	-5.47122976	0.60557418
H	5.01726213	1.63286897	-3.70762997	O	-5.62269984	-4.14157754	2.05496588
H	3.42436516	0.09530475	-3.96615152	C	-6.53419523	-2.65282594	-1.18763665
H	3.82420792	3.84070382	-4.27128915	C	-6.67380635	-1.54238338	-2.24608910
H	1.85031957	4.82960953	-5.34470853	C	-6.08790554	-0.25711264	-1.65837309
H	2.40121199	5.47348615	-2.66540674	C	-6.67174067	0.09748887	-0.27569718
H	0.23819775	3.89730612	-2.92341227	C	-6.73462372	-1.15079103	0.64803251
H	-1.47003687	4.55642412	-4.51876299	C	-7.56479698	-1.03511193	1.93613517
H	0.06528124	2.81549925	-5.76999069	O	-6.00048892	-1.92530162	-3.44058309
H	1.31959947	1.28406668	-3.40606140	O	-6.15429580	0.82918608	-2.58616926
H	1.30324547	0.89270061	-6.45740811	O	-5.75778568	1.07701434	0.21460140
H	0.30032514	-0.03638413	-5.29107305	O	-7.28207043	-2.27941680	-0.05181723
H	2.01360777	-1.31856408	-5.01684232	O	-7.03032432	-1.82777985	2.98664702
H	-1.91951971	2.20471464	-6.04390348	C	-6.12253144	1.92815091	1.27708401
H	-4.17645940	2.32145363	-5.28279944	C	-5.42067992	3.27445692	0.99476273
H	-2.67868585	3.54107627	-3.20523041	C	-3.92275313	3.21756642	1.34167507
H	-3.33724152	1.44361586	-2.47926815	C	-3.69979342	2.64267228	2.74659020
H	-5.34631363	2.67926141	-2.91428618	C	-4.34629027	1.23668233	2.74783361
H	-4.59004623	-0.29511888	-4.67241632	C	-4.17573273	0.43001968	4.03581955
H	-1.83874019	-0.11198090	-3.30619813	O	-5.60584600	3.70526412	-0.34598611
H	-1.49374747	-1.97835320	-5.29671362	O	-3.38491305	4.53965888	1.23949504
H	-3.05190561	-2.51282336	-4.56517783	O	-2.30486629	2.58824551	3.02700117
H	-1.53621886	-3.35190638	-3.10282849	O	-5.76709671	1.41199031	2.53418299
8c_gamma-CD_P:							

C	4.68981854	4.43719712	-2.71288653	C	-1.84809225	3.26616476	4.19771789
C	3.98594138	3.88645177	-3.97323934	C	-1.78689269	4.80526273	4.02345094
C	3.70168158	2.38979381	-3.74354139	C	-0.77635151	5.15263284	2.92401971
C	4.98237751	1.66231288	-3.30978997	C	0.60013213	4.57743222	3.23831802
C	5.75751720	2.35509822	-2.17754246	C	0.47890253	3.06470158	3.57032947
C	7.15846976	1.77811625	-1.96466692	C	1.75953657	2.51888422	4.23009494
O	2.85417055	4.65454675	-4.29165681	O	-3.02366701	5.45496414	3.76526496
O	3.15995708	1.81279153	-4.91160266	O	-0.71153515	6.58971699	2.79723816
O	4.56465453	0.36486971	-2.86191476	O	1.49827106	4.65634630	2.11869023
O	5.92872981	3.76807178	-2.47575013	O	-0.57078975	2.80433844	4.52449914
O	7.93509436	1.78701348	-3.15442949	O	2.90257620	2.60905839	3.40203562
C	5.33854710	-0.76540914	-3.22219109	C	1.97810592	5.93739178	1.70382273
C	4.45982907	-1.70567564	-4.06803924	C	1.39228825	6.31005807	0.31506255
C	3.30019197	-2.24745368	-3.22270379	C	1.91248101	5.31558523	-0.72112805
C	3.85536364	-2.90228498	-1.95731956	C	3.43962440	5.30254179	-0.74384197
C	4.76016180	-1.91664484	-1.18987383	C	3.99680865	5.05372460	0.67968876
C	5.45731784	-2.56114633	0.00740338	C	5.51537570	5.29216429	0.82724005
O	3.96725245	-1.00159988	-5.20368375	O	-0.01657896	6.29112985	0.22887354
O	2.48944795	-3.10673186	-4.01048797	O	1.43905535	5.64569225	-2.02417374
O	2.75637847	-3.29979702	-1.14562367	O	3.82793506	4.24297037	-1.61311625
O	5.80378004	-1.44290127	-2.07537795	O	3.38182545	5.93498259	1.64177300
H	4.93799514	5.50911074	-2.84688154	O	6.31554750	4.27978674	0.26650226

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

H	4.68683256	3.97773350	-4.82731376	H	2.89467761	3.49358584	2.98083020
H	2.99101212	2.32002515	-2.89318112	H	1.71248028	6.70142469	2.45851090
H	5.64330648	1.57169597	-4.19425053	H	1.79490375	7.32117665	0.06972364
H	5.18443372	2.26110925	-1.23709293	H	1.56299166	4.30294087	-0.42642661
H	7.06316745	0.72348377	-1.64548177	H	3.80452855	6.27926083	-1.12847934
H	7.64516054	2.34599790	-1.13902498	H	3.78938708	3.99638896	0.93641993
H	2.30605609	4.77718812	-3.47915737	H	5.72522467	5.31095234	1.91483483
H	3.31101289	0.83810531	-4.87082867	H	5.75666914	6.30776164	0.42644937
H	7.94793169	2.71175395	-3.47183240	H	-0.38422202	6.65330403	1.07661466
H	6.24403628	-0.45432374	-3.77808228	H	0.46385264	5.70040367	-1.96268404
H	5.09241693	-2.56372894	-4.38984342	H	6.26869682	4.31435350	-0.71541086
H	2.67411646	-1.38286727	-2.92297241	C	-0.22158237	0.54970307	-1.64225270
H	4.47316790	-3.77567684	-2.24068486	C	-1.67492670	1.11186506	-1.51183680
H	4.15481554	-1.06207721	-0.83173780	H	-2.07376373	0.80633760	-0.52454306
H	4.69580090	-2.84968488	0.75301791	C	0.33617724	1.01160820	-3.02577191
H	6.11454000	-1.79904934	0.47982308	H	1.36933212	0.63798047	-3.17931857
H	3.26073141	-1.56933671	-5.57943610	C	0.32923806	2.55181306	-3.11978126
H	2.63298229	-4.03721749	-3.69644081	H	0.94843461	2.98371036	-2.30917816
H	6.78975808	-3.48079096	-1.06580110	H	0.78751334	2.86791694	-4.07608970
H	3.81105492	-4.89060751	-0.30996507	C	-1.69521101	2.65348389	-1.62581022
H	2.32868153	-6.65338869	-1.12059092	H	-2.74590883	3.00954843	-1.53990045
H	0.61472112	-4.45213290	-2.38334590	H	-1.12449077	3.10880353	-0.79224561
H	0.02183139	-6.27609518	0.01559862	C	-1.11423629	3.08098339	-2.99152437
H	0.60549564	-3.25784721	-0.17522073	H	-1.10794670	4.18930371	-3.06763745
H	-0.53729699	-4.93970573	2.06221269	C	-1.98215907	2.48641898	-4.12176841
H	0.77007311	-3.75694757	2.44297451	H	-1.58172431	2.79506659	-5.10993385
H	2.43876675	-6.26633179	-3.41834616	H	-3.02285993	2.86953694	-4.04594226
H	-0.70459204	-6.35731060	-2.83555031	C	-2.54715867	0.49509236	-2.63976735
H	-1.43151631	-2.82772384	2.44010499	H	-3.57657114	0.89555719	-2.53738726
H	-2.01501221	-6.87686203	-0.30067856	C	-0.54013929	0.39254573	-4.15133703
H	-4.14256256	-6.66161117	-1.55726683	H	-0.11354642	0.71190648	-5.12480102
H	-3.15546749	-3.82655799	-2.18004061	C	-1.98142457	0.94761416	-4.01422926
H	-5.49909809	-4.80394599	-0.44199521	H	-2.61308249	0.51838564	-4.82248725
H	-2.83196546	-3.43821729	0.28638015	C	-2.56295422	-1.04374312	-2.53790274
H	-4.28640165	-2.61427593	1.94225833	H	-3.23306288	-1.47186784	-3.31295619
H	-3.59940926	-4.08355736	2.64462907	H	-2.97014561	-1.36051073	-1.55608795
H	-3.11253157	-6.05439567	-3.69289578	C	-0.55099265	-1.14795712	-4.06286158
H	-5.12336746	-3.71127981	-3.32076555	H	0.47178413	-1.55910515	-4.18495715
H	-5.63688439	-5.11184558	2.15398713	H	-1.17244130	-1.56205899	-4.88604488
H	-6.97158197	-3.60126493	-1.55473787	C	-0.25676649	-1.00893461	-1.56889163
H	-7.76241391	-1.40664630	-2.44427184	H	-0.65143007	-1.31836952	-0.58046126
H	-5.01126686	-0.43096626	-1.50663252	H	0.77367096	-1.40721448	-1.65077664
H	-7.68881539	0.54162710	-0.39497269	C	-1.12892703	-1.58369287	-2.69982263
H	-5.68606568	-1.35545660	0.93145787	H	-1.12563396	-2.68989260	-2.61917650
H	-8.60994012	-1.33315245	1.68961052	C	0.62738577	0.98583585	-0.43820070
H	-7.57422724	-0.00126941	2.31610953	C	2.88904784	1.27991930	0.51129651
H	-5.65893114	-1.11007216	-3.86226657	H	2.47189235	2.15778319	1.03687963
H	-7.09733017	1.04240339	-2.74049373	H	3.87221605	1.53790025	0.08994138
H	-6.76044744	-2.71657035	2.64178770	C	3.12675907	0.16991101	1.56269771
H	-7.22364653	2.06735453	1.30174628	C	1.80024546	-1.06129977	3.30146440
H	-5.88212105	4.04406533	1.64419776	C	2.87359456	-1.67305910	3.99249731
H	-3.39975758	2.55559457	0.62196849	C	0.47620028	-1.34015607	3.70345502
H	-4.23124039	3.26416490	3.49479911	C	2.61023217	-2.52254635	5.08625866
H	-3.91721446	0.63620230	1.91929512	H	3.89962644	-1.47512702	3.67600406
H	-4.75545265	0.93751690	4.84671392	C	0.22508886	-2.21776123	4.77380989
H	-3.10152514	0.46122071	4.30739275	H	-0.36072888	-0.88976735	3.15769503
H	-5.45034844	2.91418597	-0.91045946	C	1.28992173	-2.79273179	5.49095616
H	-3.69926826	4.90815776	0.38642969	H	1.10910594	-3.47123297	6.33147990
H	-5.48080302	-1.03097007	3.64591931	O	0.10781754	1.29757980	0.64668256
H	-2.49935442	3.00834849	5.06108771	O	4.22880329	-0.32697607	1.75293466
H	-1.42492777	5.21015487	4.98975430	C	3.71373580	-3.18412825	5.85759941
H	-1.12208551	4.71145057	1.97058173	C	-1.18182129	-2.63225879	5.03089721
H	1.02833872	5.12714585	4.10698588	O	4.94865106	-2.86250273	5.38689586
H	0.27038924	2.53174493	2.62292485	H	5.59270273	-3.34244580	5.95245509
H	1.60277554	1.44923745	4.46675147	O	-1.43599213	-2.95821306	6.31555523
H	1.90010190	3.06091875	5.19723844	H	-2.37576886	-3.24927668	6.34914305
H	-3.28287257	5.23847654	2.82998978	O	-2.04173925	-2.71561538	4.16194589
H	-1.61305210	6.90733867	3.03397425	O	3.54643381	-3.93003479	6.80401128

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

N	1.98367826	0.91726206	-0.57374268	O	6.64335867	12.22451963	-2.20293715
H	2.39921457	0.61787880	-1.45504976	O	4.04646127	11.47861677	-3.50070239
N	1.97075845	-0.16987797	2.23632416	O	4.13275437	8.83963055	-4.46240282
H	1.12856968	0.33529983	1.92061371	O	7.59790602	9.96333908	-4.94134456
8c_gamma-CD_S:				O	7.74120699	7.29264745	-6.10010937
C	0.25125966	0.68144447	0.20952483	C	3.11354083	8.60452251	-5.41503351
C	0.25888242	0.78894569	1.75101666	C	1.77040147	8.93636259	-4.71847039
C	1.71999303	0.77201294	2.23574546	C	1.46971967	7.90869235	-3.60247812
C	2.45755296	-0.43035762	1.61100410	C	1.60613484	6.47990466	-4.17402249
C	2.30748096	-0.55421979	0.08617751	C	3.00787027	6.32096817	-4.80204657
C	2.80251654	-1.89748933	-0.45860179	C	3.27909284	4.91223909	-5.35134093
O	-0.48982673	1.90644718	2.15258214	O	1.78237607	10.29244132	-4.24932547
O	1.75887390	0.68828618	3.64208852	O	0.14019723	8.08186766	-3.09815932
O	3.84672165	-0.28050581	1.92902083	O	1.45092851	5.46945911	-3.18400333
O	0.90075554	-0.49009630	-0.26408752	O	3.14089063	7.27835604	-5.87059376
O	2.10924538	-2.99197876	0.11759101	O	3.58084781	4.00815765	-4.30523146
C	4.49816249	-1.26395405	2.68105983	C	0.11761083	5.10168378	-2.80011122
C	5.35376964	-0.55769432	3.75436378	C	-0.02910946	5.29229468	-1.26358303
C	6.45017979	0.27683098	3.07160502	C	0.63925712	4.16399249	-0.47612053
C	7.27659196	-0.66128767	2.19063839	C	0.19360406	2.80779225	-1.02582380
C	6.35873607	-1.35198577	1.16121529	C	0.49356481	2.73243061	-2.53711000
C	7.09794428	-2.36263841	0.28349558	C	0.06083827	1.41536889	-3.21937475
O	4.52154083	0.25555992	4.56824242	O	0.53203451	6.51035911	-0.82905288
O	7.21464076	0.98625240	4.03465773	O	0.31277983	4.26450079	0.90702640
O	8.29945392	0.08253805	1.53827464	O	0.91725400	1.80364573	-0.33257816
O	5.33483030	-2.08041499	1.86405850	O	-0.19322055	3.80018137	-3.21543305
O	7.77717347	-3.34760559	1.04788371	O	0.96479359	0.35399802	-3.02276448
C	9.59075490	-0.49912628	1.51595037	H	-0.79351504	0.61980944	-0.15666410
C	10.44951441	0.01067769	2.69685519	H	-0.24855570	-0.10697376	2.16417402
C	10.74776688	1.50314412	2.56253216	H	2.20967202	1.70282535	1.86332199
C	11.32172713	1.80677493	1.17274101	H	2.05554332	-1.35565165	2.06889028
C	10.39428033	1.24683897	0.08604577	H	2.84714571	0.27882767	-0.40777782
C	10.90757202	1.40360343	-1.34192570	H	3.86913276	-2.02121911	-0.19521341
O	9.78531279	-0.25613598	3.93838261	H	2.70604641	0.67123911	3.91442563
O	11.63647119	1.85155850	3.60662817	H	1.15683351	-2.81273875	-0.01679979
O	11.40939224	3.22655005	1.05582883	H	3.77532063	-1.96124830	3.14886225
O	10.21815312	-0.17055068	0.30166963	H	5.84243344	-1.34749127	4.37051512
O	9.91653287	1.04544317	-2.28690753	H	5.94389814	1.02132464	2.42845603
C	12.65001387	3.84511188	0.85253985	H	7.72115362	-1.44961465	2.82992886
C	12.77112751	5.01180622	1.85507188	H	5.90014842	-0.57511533	0.51290007
C	11.72463070	6.07568668	1.52992027	H	7.86249176	-1.82822844	-0.31181087
C	11.87248649	6.49052748	0.06094878	H	6.36382198	-2.82083595	-0.42013707
C	11.75628614	5.27053142	-0.86743400	H	5.11999806	0.88602165	5.02144371
C	11.98040884	5.59141185	-2.34506967	H	8.11043466	0.56777625	4.08713851
O	12.62369086	4.51604613	3.18181797	H	7.11058920	-3.73566806	1.65036562
O	11.92334801	7.16118338	2.42243645	H	9.52056023	-1.60416596	1.53902141
O	10.86736205	7.46061800	-0.23066669	H	11.41372593	-0.54174840	2.66661555
O	12.77862363	4.32425632	-0.47729615	H	9.78214577	2.05105991	2.65069926
O	13.15194259	6.36437201	-2.57834759	H	12.32711048	1.34228106	1.08609946
C	11.30238876	8.79134742	-0.33389528	H	9.41326100	1.75379079	0.16259646
C	10.26072640	9.71497123	0.33204194	H	11.17218443	2.46234859	-1.51999388
C	8.95940879	9.76230152	-0.47894727	H	11.83922939	0.79543816	-1.45110227
C	9.24106548	10.05569499	-1.96150990	H	10.32854960	0.19055868	4.62235825
C	10.30212112	9.06144938	-2.47884800	H	11.85754320	2.81256642	3.52056367
C	10.74389166	9.24139994	-3.93126551	H	9.61232275	0.14924541	-2.03952966
O	10.03433197	9.28273412	1.66587046	H	13.48498751	3.12944569	0.99337594
O	8.03625337	10.68546085	0.11729706	H	13.77916862	5.46593562	1.72762555
O	8.00852430	9.91360820	-2.64682768	H	10.71696633	5.62555795	1.66435389
O	11.49055635	9.18222280	-1.67560829	H	12.87892466	6.92444408	-0.10133546
O	11.54334342	8.16597521	-4.37272704	H	10.75439870	4.80797240	-0.75468749
C	7.75273041	10.73657994	-3.78020142	H	11.13798455	6.18913938	-2.73234972
C	6.49034644	11.57203055	-3.45047245	H	12.00278246	4.63126099	-2.90805997
C	5.23257783	10.68686730	-3.48693370	H	12.43967487	5.29681889	3.74477816
C	5.19282471	9.75879310	-4.70791366	H	11.18557630	7.80223359	2.29415978
C	6.52042699	9.00498060	-4.86886023	H	13.91943723	5.83573814	-2.28559845
C	6.60711329	8.13590985	-6.12178578	H	12.28266058	8.92619274	0.16293718

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H	10.70537868	10.73926506	0.32304049	H	5.08093353	3.05295604	2.02258770
H	8.46199322	8.77870130	-0.41205099	H	6.15975345	4.15516141	2.92346065
H	9.63118241	11.09503128	-2.05761817	C	7.05724951	3.33748955	1.11263806
H	9.87638609	8.04308167	-2.37298800	H	7.51437452	2.49164004	1.65851767
H	11.26385270	10.22805631	-4.02081581	C	3.95562668	5.47644873	2.02038688
H	9.84564436	9.25999627	-4.57501075	O	2.79591406	5.17543051	1.72765411
H	9.19514055	9.68750959	1.96706696	N	4.25173929	6.15864762	3.17098544
H	8.42819896	11.58224378	0.06040840	H	5.22494020	6.33735675	3.40860475
H	12.27109311	8.02302969	-3.72991196	C	3.25211237	6.65370205	4.10433321
H	8.61230301	11.40798124	-3.97183747	H	2.27010090	6.46984098	3.64425462
H	6.37850742	12.36251352	-4.21701331	H	3.30531498	6.11346880	5.07068232
H	5.24834546	10.02968172	-2.59030130	C	3.59306020	8.12652868	4.40264770
H	4.99127195	10.36520509	-5.61769594	O	4.45839623	8.39661516	5.22603364
H	6.66513384	8.35025701	-3.98873907	N	3.01105451	9.13260619	3.64324879
H	6.58515767	8.80301378	-7.01891690	H	3.47510628	10.03079136	3.79755409
H	5.71454539	7.48197834	-6.15884141	C	2.07632516	9.09228205	2.57628341
H	6.78762817	11.51596014	-1.53545229	C	0.88308884	8.34423966	2.65342474
H	3.72460700	11.58144118	-2.56556024	C	2.34675288	9.83532500	1.41172205
H	8.53383965	7.86207141	-6.05039207	C	-0.01539452	8.32779021	1.57325669
H	3.24998678	9.24673359	-6.30910826	H	0.64381796	7.76851081	3.55164301
H	0.95726323	8.85827777	-5.46695192	C	1.41663399	9.86565609	0.35123074
H	2.21295379	8.02394107	-2.78506038	H	3.29259403	10.38169913	1.30489378
H	0.85024875	6.34502036	-4.97953367	C	0.22217181	9.13105999	0.44728779
H	3.77575349	6.52561032	-4.03157550	H	-0.50848739	9.12102231	-0.36634276
H	4.16647348	4.96561625	-6.01229930	C	1.81012611	10.54521289	-0.92167159
H	2.41071794	4.57639671	-5.96789236	O	2.92280375	11.04166866	-1.08879484
H	2.72721742	10.62469049	-4.09814326	O	0.85782273	10.52017333	-1.86567134
H	0.08959753	8.97016168	-2.67959541	H	1.24110320	10.63744777	-2.82043622
H	2.85036845	4.09386083	-3.65861283	C	-1.17701082	7.37668356	1.51936243
H	-0.60092021	5.75662312	-3.32593917	O	-2.03174560	7.37670273	0.65681326
H	-1.12101935	5.25505913	-1.04179209	O	-1.12833754	6.47215657	2.52962612
H	1.73574483	4.24051179	-0.61030225	H	-1.80223380	5.78288047	2.33901155
H	-0.89918026	2.68975089	-0.86226766				
H	1.59096264	2.81592589	-2.68153871				
H	0.02907890	1.62415665	-4.30753782				
H	-0.98078921	1.16523493	-2.89971682				
H	0.25695739	7.19112722	-1.48465786				
H	1.05308835	4.74117580	1.34806952				
H	0.89097707	0.02023367	-2.10100609				
C	5.17768015	5.06157015	1.17075935				
C	4.72628189	4.62001445	-0.25652680				
H	3.97631606	3.81201405	-0.14398418				
C	6.21976815	6.21945422	0.98569131				
H	6.58446943	6.57052150	1.97560849				
C	5.58212590	7.40093403	0.21660331				
H	4.70573373	7.79278446	0.77567229				
H	6.31236914	8.23329101	0.13526168				
C	4.10878635	5.79781312	-1.04362671				
H	3.80635088	5.42898131	-2.04031680				
H	3.19325890	6.16938085	-0.54826138				
C	5.14642054	6.93158395	-1.19009459				
H	4.69574415	7.78129704	-1.74439984				
C	6.37989972	6.40588597	-1.95887195				
H	7.13617926	7.21326026	-2.06428772				
H	6.08655033	6.08944370	-2.98096224				
C	5.95835681	4.06761552	-1.03232905				
H	5.61394989	3.74525625	-2.03596035				
C	7.45215348	5.66319703	0.21505800				
H	8.20233996	6.47687985	0.11525337				
C	6.99555363	5.21406404	-1.19735822				
H	7.87556246	4.82774407	-1.75477717				
C	6.59454779	2.87761857	-0.28596485				
H	7.45043594	2.47679502	-0.86933499				
H	5.85360870	2.05551254	-0.18145035				
C	8.08239547	4.48161433	0.97738881				
H	8.41755824	4.81154113	1.98455832				
H	8.98347293	4.12036126	0.44438885				
C	5.84000170	3.85384245	1.90415133				

9c_beta-CD_P:

C	0.23842953	5.74497560	2.20793781
C	-0.37116981	5.22260966	3.52063592
O	0.54571362	5.23767738	4.60253981
C	-0.91020234	3.80199758	3.28570165
O	-1.53567246	3.31038129	4.46948288
C	-1.88181125	3.74825989	2.10232682
O	-2.14288229	2.38565320	1.79481665
C	-1.20457817	4.40158983	0.86813122
O	-0.72222949	5.72129215	1.17049725
C	-2.16936147	4.50529137	-0.30307814
O	-1.44613795	4.89168786	-1.48258066
C	-3.49732432	1.93818443	1.66536740
C	-4.13237409	1.66387854	3.05412370
O	-4.19846313	2.83900623	3.82938046
C	-3.37087967	0.50399976	3.70439588
O	-3.98065000	0.15537529	4.93140292
C	-3.34202749	-0.69845357	2.73291588
O	-2.57434310	-1.72390743	3.35571081
C	-2.73993604	-0.32128727	1.36086229
O	-3.48343897	0.80665933	0.84397234
C	-2.84227985	-1.40113991	0.25671261
O	-1.87378252	-2.42832598	0.34577013
C	-3.27630124	-2.72960156	4.05316036
C	-2.47549823	-3.09760241	5.31627732
O	-2.31979279	-1.94290314	6.13643031
C	-1.12593061	-3.65018146	4.88064334
O	-0.40501208	-4.07035146	6.03744077
C	-1.23979894	-4.77900660	3.83837886
O	0.13659008	-4.90840422	3.41945844
C	-2.21010979	-4.37812424	2.70245900
O	-3.44031036	-3.88550059	3.27286327
C	-2.63729132	-5.45591299	1.69328630
O	-3.22946827	-4.88780276	0.54273912

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C	0.53377509	-5.96458541	2.60303021	H	0.44980581	-4.41646253	5.70639138
C	1.98555588	-6.36200321	2.98978440	H	-1.56482749	-5.71968359	4.33775102
O	2.19013459	-6.47141330	4.39722497	H	-1.71506429	-3.56143819	2.14918430
C	3.01184048	-5.34483889	2.48001008	H	-3.39679277	-6.10607547	2.17742866
O	4.33295912	-5.85286075	2.63712555	H	-1.76576906	-6.08700746	1.42316363
C	2.76132997	-5.05656533	0.99655953	H	-2.67653907	-4.11413959	0.27692063
O	3.75866973	-4.15276231	0.55385064	H	-0.14148855	-6.83872865	2.72881994
C	1.31515164	-4.53714081	0.83691460	H	2.20712703	-7.32567921	2.47913103
O	0.46713046	-5.64206515	1.22345356	H	1.69985118	-7.24802870	4.72737360
C	0.90499862	-4.05484161	-0.57810282	H	2.88737471	-4.39569089	3.04900246
O	0.66877120	-2.65032087	-0.60266801	H	4.42414310	-6.12324393	3.57280223
C	4.43801754	-4.43304879	-0.65979650	H	2.83745731	-6.01127230	0.43454666
C	5.95356358	-4.33197104	-0.38826565	H	1.14612495	-3.68490843	1.52155650
O	6.38682957	-5.18208907	0.65332053	H	1.67185152	-4.32892118	-1.32920840
C	6.34011376	-2.86984095	-0.12032578	H	-0.04156369	-4.57876381	-0.82766525
O	7.75021167	-2.72396253	-0.02003745	H	1.31168942	-2.14041257	-1.16994920
C	5.82808444	-1.96460489	-1.24159455	H	4.18631807	-5.45177879	-1.01683582
O	6.16277190	-0.63435252	-0.85683394	H	6.48199254	-4.65545390	-1.30797036
C	4.29856378	-2.16363982	-1.39374222	H	5.71271815	-5.16918454	1.37603125
O	4.03894276	-3.55478454	-1.68264124	H	5.84420840	-2.54679329	0.82394279
C	3.60749033	-1.33059957	-2.48258904	H	8.05421617	-3.44089780	0.57535696
O	2.28214574	-0.95582480	-2.10273910	H	6.33740326	-2.23372464	-2.19213805
C	6.75054893	0.24733503	-1.78704914	H	3.82680314	-1.90252473	-0.42989617
C	7.81726025	1.06041078	-1.02565207	H	3.55018140	-1.95024296	-3.40139803
O	8.76511309	0.22974826	-0.39406066	H	4.21233687	-0.43341935	-2.71065259
C	7.12400359	2.01260570	-0.03783971	H	2.28543027	0.00108378	-1.83464939
O	8.11374287	2.90107166	0.47878622	H	7.21593735	-0.31076711	-2.62403518
C	5.96033354	2.79819021	-0.66934840	H	8.36332870	1.68083821	-1.76422865
O	5.30445539	3.489444949	0.40788112	H	8.30305874	-0.57598660	-0.06348147
C	5.00818162	1.81837699	-1.38985954	H	6.69386675	1.39777425	0.78337706
O	5.78653454	1.09915118	-2.36963806	H	7.71781520	3.31010476	1.28501189
C	3.79178425	2.41403772	-2.11336339	H	6.36159507	3.52484708	-1.40556748
O	2.59854072	1.84148162	-1.57704589	H	4.61866766	1.10984775	-0.63179886
C	5.19105364	4.89518128	0.33054449	H	3.89294117	2.18282309	-3.19673329
C	5.03914553	5.44259875	1.77269805	H	3.78251978	3.51559299	-2.00666909
O	6.10080129	5.10091754	2.63880091	H	1.89208017	2.54518487	-1.59797622
C	3.68298769	5.00215017	2.34264621	H	6.08904128	5.33181342	-0.15104432
O	3.44386057	5.53126660	3.64118813	H	5.05058915	6.54747465	1.70023572
C	2.55306018	5.43752447	1.41288144	H	6.17670776	4.12462743	2.70754486
O	1.34020748	4.90785243	1.93140776	H	3.67914452	3.89385302	2.37418484
C	2.81009141	4.86265307	0.00591107	H	4.25846474	5.37815790	4.16547762
O	4.09711810	5.30723502	-0.47041961	H	2.51167337	6.54695646	1.37026259
C	1.74433217	5.25122376	-1.03621717	H	2.81067921	3.76004942	0.10487934
O	1.11574961	4.08683798	-1.57431326	H	2.25481211	5.82604719	-1.83974421
H	0.55598298	6.80224476	2.30745283	H	0.97299286	5.89974187	-0.57660998
H	-1.21728935	5.88255823	3.79892670	H	0.14311597	4.26946846	-1.66192581
H	1.45491339	5.07447599	4.25496581	C	2.09915069	1.64204772	3.14748247
H	-0.05495590	3.15487392	3.02360972	C	1.37681130	1.06508237	4.39686891
H	-0.94343144	3.54875503	5.21368214	H	0.29610873	1.31239963	4.34512940
H	-2.81409223	4.28885606	2.36135489	C	3.60974120	1.30266633	3.25651775
H	-0.35424129	3.75611513	0.57023802	H	4.14467961	1.72038683	2.37777143
H	-2.95211906	5.25882433	-0.06816253	C	4.20289076	1.90422312	4.53762334
H	-2.63952240	3.51036597	-0.44677629	H	4.10179020	3.00519141	4.53821836
H	-2.05406059	4.89797254	-2.24498211	H	5.28442845	1.67275792	4.59166624
H	-4.10252808	2.70369123	1.13351283	C	1.96498697	1.68262657	5.68538430
H	-5.17843893	1.33753165	2.87497517	H	1.43306878	1.28852244	6.57754094
H	-3.32714527	2.96646552	4.27321877	H	1.83180196	2.78440033	5.66953736
H	-2.31704918	0.82711233	3.85985311	C	3.48139990	1.34101423	5.79203887
H	-3.35202842	-0.41821182	5.42552824	C	3.63515013	-0.20634146	5.79381496
H	-4.38366838	-1.04423077	2.56111299	H	4.70752408	-0.47624947	5.89705430
H	-1.67391224	-0.04146353	1.48805358	H	3.08474563	-0.65341260	6.65092721
H	-2.78609911	-0.86493884	-0.71711241	C	1.53998180	-0.47945660	4.38722091
H	-3.83246927	-1.89581058	0.31797391	H	1.00421462	-0.91124326	5.26121226
H	-0.99532828	-2.21166274	-0.06540827	C	3.78095490	-0.23782574	3.25222107
H	-4.29123872	-2.38697114	4.32961265	H	4.86359890	-0.48218516	3.31925635
H	-3.04614145	-3.88755446	5.85326309	C	3.05343453	-0.80838961	4.49800813
H	-1.61830231	-2.14448730	6.78669707	H	3.18409638	-1.91245480	4.52187022
H	-0.59720324	-2.81721263	4.37814078	C	0.96109803	-1.07394826	3.08749035

Electronic Supplementary Information: Nanodiamonds in Sugar Rings

H	1.08449380	-2.17589098	3.10126949	O	-0.20031159	-3.48512571	5.43157523
H	-0.12703970	-0.87457130	3.03516840	C	-1.23633265	-3.84211246	3.22854557
C	3.19036355	-0.82228732	1.95581184	O	0.05399836	-3.96037935	2.60457985
H	3.73063522	-0.38856956	1.08872538	C	-2.30805097	-3.24812903	2.28099062
H	3.33806698	-1.92160657	1.92125773	O	-3.53218804	-3.09757932	3.02711786
C	1.50603911	1.05130595	1.85204284	C	-2.59185172	-4.12759085	1.06007024
H	0.42696098	1.30353193	1.77760483	O	-3.59642102	-3.64105334	0.19848504
H	2.01053940	1.48806874	0.96468418	C	0.66118976	-5.22916340	2.48735094
C	1.68656000	-0.48230839	1.86072604	C	2.08950662	-5.18263339	3.09160103
H	1.26863982	-0.92561833	0.93864754	O	2.13493231	-4.70381239	4.44342597
C	4.10230930	2.02391635	7.02936302	C	2.99701852	-4.27068747	2.26574566
C	4.96823900	1.71518679	9.33930993	O	4.33546963	-4.32316497	2.75026229
H	4.86735561	2.81150426	9.45022996	C	2.98459120	-4.72507296	0.80461795
H	4.60907886	1.20979502	10.25243830	O	3.74433197	-3.78988711	0.04511658
C	6.44129901	1.29346138	9.08740341	C	1.53213468	-4.81792641	0.28445278
C	7.96540020	1.55446365	7.13313847	O	0.75292747	-5.67181765	1.15245684
C	8.97147859	0.62050512	7.46204730	C	1.41099458	-5.39154133	-1.14590749
C	7.84868956	2.00474428	5.80255063	O	1.56478465	-4.43169016	-2.16490655
C	9.83325333	0.14144318	6.45081616	C	4.69852072	-4.26884631	-0.89790062
H	9.06707153	0.26429285	8.48982645	C	6.11613926	-3.89853396	-0.41777494
C	8.68971321	1.50137801	4.79480233	O	6.42649347	-4.42528399	0.85489015
H	7.07341377	2.73070140	5.52971885	C	6.29201369	-2.37350457	-0.45728267
C	9.69459412	0.57013634	5.11663761	O	7.60485771	-2.00404731	-0.06516313
H	10.36147314	0.16973700	4.34524805	C	6.03305446	-1.85724061	-1.86935196
O	4.55624241	3.17448108	6.97871166	O	6.07832043	-0.43307030	-1.78939100
O	6.97011150	0.34903682	9.65082948	C	4.65408906	-2.32237096	-2.39828027
C	10.92484582	-0.84397033	6.74805366	O	4.43780590	-3.74790923	-2.17838754
C	8.42370782	1.95015715	3.39273351	C	4.49636230	-2.08881465	-3.91757591
O	10.98670350	-1.17666158	8.06686863	O	3.17130291	-1.82806152	-4.31874967
H	11.72838229	-1.81508050	8.15401939	C	6.63967741	0.33923468	-2.83663712
O	9.29537073	1.49689823	2.49657463	C	7.53442580	1.41083066	-2.17884026
H	9.04358887	1.83476823	1.57640029	O	8.51866742	0.80814299	-1.37263959
O	7.45402559	2.66074674	3.11014430	C	6.66569998	2.43949354	-1.42234039
O	11.68582829	-1.30722441	5.92058484	O	7.46756200	3.56543188	-1.11812139
N	4.15923724	1.29293150	8.19143934	C	5.41201219	2.86869514	-2.22457514
H	3.91143825	0.30719083	8.15556996	O	4.47969278	3.48718515	-1.31724350
N	7.01008363	2.03056995	8.05537667	C	4.68969737	1.69924763	-2.91642462
H	6.39559953	2.76320549	7.67904906	O	5.64114111	0.91814839	-3.64868646
H	1.98291887	2.74302544	3.14722792	C	3.63355850	2.18301656	-3.91103146
9c_beta-CD_S:							
C	-0.08192841	5.99139659	1.45090339	O	2.82462985	1.11271444	-4.40388119
C	-0.34328209	5.70164650	2.94285760	C	4.43735507	4.89944410	-1.21814397
O	0.80921188	5.78772644	3.75463422	C	4.54329164	5.24431496	0.29044040
C	-1.01474087	4.32190492	3.08108317	O	5.63241616	4.55857912	0.92439801
O	-1.23176721	4.02842671	4.45649280	C	3.24418746	4.92383513	1.03580102
C	-2.32298115	4.32101386	2.28218663	O	3.27549742	5.45792890	2.35666367
O	-2.92080857	3.02919734	2.32072770	C	2.03058999	5.48140423	0.29668004
C	-1.96895955	4.65489406	0.80714061	O	0.87756497	5.05009540	1.00231230
O	-1.27467029	5.91511975	0.71210547	C	2.05007790	4.97025209	-1.15899706
C	-3.18739247	4.74077696	-0.11665958	O	3.26601049	5.44571112	-1.78278807
O	-2.85575325	4.43595601	-1.47134856	C	0.81311951	5.37214863	-1.98535203
C	-4.24648969	2.87727570	2.80364209	O	-0.08247232	4.27777679	-1.99497486
C	-4.27766144	2.57352683	4.32326873	H	0.29567053	7.02564037	1.31848104
O	-3.86883865	3.69278624	5.06182268	H	-1.05446399	6.46641931	3.31638111
C	-3.47091496	1.28466830	4.57246169	H	1.59411064	5.45764907	3.24973031
O	-3.57277754	0.89394920	5.92197397	H	-0.34316118	3.55300219	2.64061565
C	-3.99518693	0.16159450	3.65430712	H	-0.45769138	4.39439593	4.93851539
O	-3.05067044	-0.91158648	3.72048964	H	-3.00986769	5.08426101	2.70271916
C	-4.14116293	0.55940461	2.17443486	H	-1.30799606	3.84611158	0.43508846
O	-4.85347404	1.82208256	2.07237006	H	-3.58000531	5.77753657	-0.08006700
C	-4.88776456	-0.51121153	1.35433455	H	-3.96793123	4.04397823	0.24251547
O	-4.22364010	-0.87046820	0.14556764	H	-3.10260272	3.49703849	-1.62024963
C	-3.45116168	-2.19704762	4.11824929	H	-4.84973293	3.78421569	2.59258349
C	-2.42846942	-2.72271550	5.14185462	H	-5.33619607	2.37909116	4.59339547
O	-2.33235192	-1.81061172	6.22620517	H	-2.88645142	3.78280297	4.98879599
C	-1.07542045	-2.93507218	4.45974243	H	-2.41495929	1.48461920	4.28014797
				H	-3.05170014	0.06413878	6.02711921
				H	-4.98055782	-0.16030214	4.05370116
				H	-3.12560220	0.69960304	1.76283405

H	-5.92285367	-0.15762705	1.15628433	C	1.31458617	-1.25698306	-0.69318284
H	-4.94547861	-1.45375815	1.92649298	H	1.77696400	-2.18691033	-1.07036231
H	-3.95580132	-0.06602840	-0.34205405	C	-0.78591530	-0.25561515	0.27035128
H	-4.46551459	-2.17721748	4.56421565	H	-1.82482081	-0.47890970	0.57585347
H	-2.79243628	-3.71273131	5.49774054	C	-0.14197683	-1.55838919	-0.26412134
H	-1.52137873	-2.04948815	6.72020334	H	-0.13105608	-2.30226536	0.55817255
H	-0.70878320	-1.94467586	4.10880236	C	2.12197704	-0.71236320	0.50204514
H	0.68479904	-3.58423324	5.00993104	H	2.16142220	-1.47696503	1.30515969
H	-1.58416480	-4.84110473	3.56636898	H	3.17044501	-0.51272627	0.19014259
H	-1.96833828	-2.24861019	1.94364119	C	0.01423808	0.28220428	1.47274435
H	-2.91916278	-5.12916139	1.41319795	H	-0.46684127	1.20434877	1.86255883
H	-1.61870211	-4.26203466	0.53119567	H	0.00664936	-0.46627409	2.29524150
H	-3.62861667	-2.65629583	0.19483896	C	1.44003121	1.62359451	-0.10318199
H	0.05560914	-5.99829601	3.01136076	H	2.47965538	1.85758498	-0.41575524
H	2.50411167	-6.21153083	3.04354483	H	0.97593429	2.56240135	0.25669877
H	1.84850862	-5.41990118	5.04370956	C	1.46467295	0.57979603	1.03169413
H	2.59996873	-3.23554662	2.31982155	H	2.04524531	0.97682293	1.89219688
H	4.31106377	-4.10938020	3.70390452	C	-1.79333175	-1.51719003	-3.84176451
H	3.45278714	-5.73204830	0.75980319	C	-3.12982576	-3.23935379	-5.01819305
H	1.09506599	-3.80715304	0.28628476	H	-2.72921681	-2.78004806	-5.94307921
H	2.11177122	-6.25318609	-1.26193717	H	-3.07799038	-4.33923860	-5.09225519
H	0.38150220	-5.79229416	-1.23330171	C	-4.61658144	-2.84290996	-4.81452221
H	2.50602218	-4.15667290	-2.25372289	C	-5.73365790	-0.81910977	-3.95377486
H	4.60993652	-5.36922905	-1.00226455	C	-7.06793329	-1.26550604	-3.83549910
H	6.84077513	-4.34845907	-1.12606620	C	-5.28648194	0.24355335	-3.14621071
H	5.69884615	-4.20382071	1.48814621	C	-7.92730033	-0.65657713	-2.89514889
H	5.53163393	-1.92020731	0.22082122	H	-7.41789031	-2.09794434	-4.45002561
H	7.82898067	-2.58053855	0.69607815	C	-6.12737328	0.80462275	-2.16746025
H	6.84496373	-2.23022597	-2.53117774	H	-4.24611756	0.58213599	-3.21570529
H	3.87880976	-1.75430063	-1.85064679	C	-7.45963976	0.36400801	-2.04736120
H	4.84188580	-3.01952285	-4.41663560	H	-8.12549254	0.77709844	-1.28214641
H	5.16591525	-1.26459374	-4.22897015	O	-1.99292873	-0.71021991	-4.76345992
H	3.05143938	-0.85069011	-4.35157840	O	-5.50629599	-3.65426434	-4.62882951
H	7.25122333	-0.29778842	-3.50574913	C	-9.35239722	-1.09272502	-2.72536809
H	8.06139178	1.95491417	-2.98738471	C	-5.48741012	1.67149657	-1.13815681
H	8.08385511	0.10024228	-0.84545223	O	-9.70624495	-2.07943124	-3.59295442
H	6.29746378	1.92469458	-0.50286385	H	-10.64373377	-2.29588477	-3.39444327
H	7.04048042	4.07126312	-0.39289297	O	-6.30091970	2.05622389	-0.15114317
H	5.73754048	3.59714046	-2.99585141	H	-5.73141003	2.21262844	0.66810391
H	4.20595668	1.07367164	-2.13973211	O	-4.27361570	1.90766803	-1.11946035
H	4.15860196	2.64651258	-4.77270888	O	-10.12625679	-0.62943551	-1.90959163
H	3.01724247	2.96153922	-3.41731148	N	-2.30479078	-2.78474232	-3.89572147
H	1.91939904	1.21070111	-4.05878936	H	-2.24030430	-3.39070082	-3.08095048
H	5.28299682	5.35311347	-1.76986501	N	-4.78119442	-1.45838078	-4.77493908
H	4.75702234	6.32379185	0.39604757	H	-3.90961350	-0.92913680	-4.92674400
H	5.42391814	3.60306332	0.83132195	H	0.62066072	1.86256799	-2.10488050
H	3.12261512	3.81617574	1.06802694				
H	4.12321840	5.18362299	2.76175436				
H	2.09179740	6.59132043	0.28411913				
H	2.07097158	3.86948613	-1.15595673				
H	1.17094682	5.61753592	-3.01314714				
H	0.34224522	6.28739387	-1.56449269				
H	-1.02011224	4.56178816	-1.86054539				
C	0.64127839	1.08735858	-1.31008637				
C	1.27009154	-0.22485215	-1.84604753				
H	2.30526153	-0.03003153	-2.18544902				
C	-0.81723312	0.77841704	-0.88445651				
H	-1.30150620	1.71278433	-0.53426790				
C	-1.61860872	0.22041720	-2.07156406				
H	-1.66292435	0.96160510	-2.89261442				
H	-2.65901436	0.01847755	-1.76258471				
C	0.46678065	-0.79016855	-3.03660715				
H	0.95723511	-1.70569854	-3.41420784				
H	0.42161601	-0.06459200	-3.87596901				
C	-0.98786315	-1.09614131	-2.60043958				
C	-0.94351962	-2.13041136	-1.45183877				
H	-1.96816802	-2.38127526	-1.11742969				
H	-0.44523794	-3.05736041	-1.79935995				

9c_gamma-CD_P:

C	0.39860666	-0.55171344	-0.51999768
C	0.38575757	-0.70349529	1.02117094
C	1.71898458	-0.16844346	1.59595711
C	2.89085385	-0.84424574	0.86367859
C	2.79965177	-0.63672676	-0.65606182
C	3.90489373	-1.35035430	-1.43303342
O	-0.75097783	-0.09084096	1.59777429
O	1.79903620	-0.35717995	2.99578169
O	4.11609985	-0.31884717	1.37050944
O	1.52963614	-1.19947792	-1.10191471
O	4.00720497	-2.73026204	-1.10338467
C	5.12200686	-1.25405103	1.72830010
C	4.86725950	-1.92432598	3.10178402
C	4.89695224	-0.89443078	4.22760859
C	6.16844466	-0.05718489	4.16550812
C	6.38135475	0.51183678	2.75054557
C	7.74556339	1.18796086	2.60510258
O	3.62223158	-2.63617564	3.10070794
O	4.78401620	-1.61531661	5.46540423

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O	6.02981483	1.00503399	5.10614597	O	1.82475162	0.15074766	-3.55424182
O	6.34665128	-0.56746952	1.78808999	H	-0.49249206	-1.03839679	-0.96629909
O	8.81556363	0.31565751	2.93739164	H	0.33969884	-1.79099393	1.24765431
C	7.04868121	1.21792277	6.06246091	H	1.75726476	0.92459422	1.41988470
C	6.48154116	0.95781420	7.47655438	H	2.83418531	-1.93419464	1.03855307
C	5.42864929	2.00682151	7.83406383	H	2.82698004	0.44275809	-0.90123772
C	5.97576773	3.42026439	7.60731051	H	4.87168717	-0.88315336	-1.16595761
C	6.57110418	3.57722012	6.20001447	H	3.73398425	-1.18930882	-2.52054981
C	7.32310544	4.89420515	5.99967129	H	-1.13726382	0.58428959	0.97520227
O	5.93429855	-0.36173335	7.54729133	H	2.21403594	-1.23082461	3.18208932
O	5.06512650	1.79529058	9.18075715	H	3.12625012	-3.12497261	-1.25844544
O	4.88715869	4.32795844	7.78863953	H	5.22450923	-2.03442959	0.94794775
O	7.54698186	2.53463080	5.97778193	H	5.70382966	-2.63920156	3.25941778
O	7.87041742	5.00404755	4.69756554	H	4.03159105	-0.21319777	4.10128948
C	4.88707136	5.15433129	8.92301012	H	7.03880707	-0.69544730	4.41603671
C	3.49918995	5.11951497	9.60337320	H	5.57777222	1.24003185	2.52952129
C	2.42694935	5.83442231	8.76182005	H	7.79076178	2.04273772	3.30526275
C	2.93250442	7.15376959	8.16432581	H	7.83346406	1.57977744	1.56592779
C	4.34989696	7.05144462	7.57647722	H	3.56777159	-3.10425858	3.95810282
C	4.96496460	8.40423127	7.21178475	H	5.22958671	-1.09086355	6.20794091
O	3.17580303	3.75908198	9.88984030	H	8.71874534	-0.47045361	2.36324576
O	1.28828205	6.17575171	9.55261055	H	7.91749003	0.56156770	5.85825623
O	2.01495991	7.54830675	7.14075681	H	7.32012151	1.04569375	8.20062716
O	5.22351202	6.48508402	8.57663709	H	4.56101274	1.87288196	7.15258603
O	4.89429267	9.34263339	8.27688726	H	6.77373411	3.61295848	8.35498123
C	1.08830687	8.55079324	7.47961603	H	5.76330198	3.49251481	5.44520046
C	-0.20381614	8.30367185	6.67023956	H	6.62227035	5.73745858	6.13720166
C	0.08209984	8.50267498	5.17533036	H	8.11409860	4.97130678	6.78424552
C	0.68079357	9.88585028	4.91901361	H	5.16150168	-0.31502758	8.15650223
C	1.92739939	10.04770995	5.81115375	H	4.29913295	2.38663869	9.39166695
C	2.61825195	11.40752310	5.71928169	H	8.36867886	4.17804848	4.53344638
O	-0.81232598	7.04442437	6.89625473	H	5.65758199	4.82774823	9.64911653
O	-1.11477134	8.32037930	4.40902120	H	3.59607151	5.69415603	10.55111989
O	1.07482518	9.95193601	3.55155060	H	2.14892340	5.17027964	7.91274003
O	1.58669807	9.84723134	7.19262153	H	2.96710767	7.91582829	8.96686705
O	3.87991737	11.40245328	6.35079195	H	4.33232018	6.40130890	6.67753123
C	0.66773028	11.06895053	2.77500954	H	4.43297351	8.86114457	6.36277513
C	-0.72361752	10.80753194	2.14204001	H	6.01810137	8.22220547	6.89647721
C	-0.61648488	9.61280851	1.18156734	H	2.20365389	3.61769493	9.87892432
C	0.47745217	9.88916316	0.15309914	H	0.86700469	5.33587981	9.84903917
C	1.80780499	10.16325540	0.88795072	H	5.34420506	8.94240740	9.04675248
C	2.98689381	10.48194400	-0.05246849	H	0.86825243	8.53815024	8.56242160
O	-1.77683413	10.61627716	3.06687303	H	-0.94024008	9.06466156	6.99553986
O	-1.87514264	9.38902124	0.53885387	H	0.82874313	7.74532197	4.86186454
O	0.62737754	8.75748376	-0.69962779	H	-0.06980895	10.66593431	5.16001949
O	1.62634356	11.28581650	1.77320064	H	2.64890658	9.27278294	5.48459249
O	3.57521572	9.32870501	-0.62214082	H	1.92800436	12.17924353	6.14389635
C	0.53195847	8.91638340	-2.10622708	H	2.79398637	11.64407077	4.65145139
C	-0.86845539	8.50811599	-2.60293590	H	-0.23054718	6.33812105	6.52157542
C	-1.11217004	7.04291827	-2.20473239	H	-1.62645949	7.62035535	4.87003809
C	-0.01117574	6.16399248	-2.80694972	H	3.78799103	11.00098572	7.24085232
C	1.38853218	6.69658551	-2.40287298	H	0.64369331	11.99135610	3.39211136
C	2.53446845	5.98768082	-3.14425856	H	-0.99066040	11.70917317	1.55388931
O	-1.91636977	9.34359931	-2.16601648	H	-0.33759595	8.71012800	1.76330385
O	-2.40822002	6.63841939	-2.66895400	H	0.19622961	10.78646501	-0.43813636
O	-0.08665677	4.81238412	-2.34066294	H	2.08375674	9.26337937	1.47163330
O	1.51289713	8.10212737	-2.70536107	H	3.76700220	10.97065312	0.56283762
O	2.70089017	4.65435890	-2.71389259	H	2.66052782	11.21857579	-0.82622180
C	-1.09221211	3.97812646	-2.92752452	H	-1.61252046	9.77345872	3.57004128
C	-2.02470379	3.43575607	-1.81369331	H	-2.56601649	9.64080369	1.19028303
C	-1.25613344	2.45320534	-0.93282346	H	2.92945094	8.88863077	-1.21204142
C	-0.47446340	1.41328648	-1.74279391	H	0.76458741	9.95892469	-2.40509311
C	0.30613026	2.01012303	-2.93134028	H	-0.85828382	8.57621418	-3.70969375
C	0.76914390	0.97621537	-3.98039764	H	-1.06770498	6.95599691	-1.10004364
O	-2.54279398	4.44780549	-0.97576039	H	-0.10042527	6.19020876	-3.91569208
O	-2.10868964	1.70027463	-0.08219243	H	1.51482150	6.54022748	-1.31313923
O	0.43417432	0.81847591	-0.81527294	H	3.47327257	6.53518214	-2.92922597
O	-0.51111377	2.93640905	-3.66384484	H	2.34487520	6.06022818	-4.24365459

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C	5.87824815	9.58987574	-2.15061784	H	12.94802297	7.60815776	1.29939316
C	6.59859989	9.77766087	-3.47534379	H	9.92513246	9.09216634	4.03213342
O	3.42477212	10.43440146	1.14755753	H	7.74235015	10.17009190	4.35988775
O	2.28916648	9.08735405	-1.08331259	H	6.64653104	8.10232213	2.35343985
O	4.21156464	7.95021040	-2.92082568	H	6.93492668	11.13400423	1.99593047
O	6.00408287	10.83765831	-1.43977691	H	8.45400012	8.75741735	0.77265523
O	7.98707355	9.83620673	-3.22634008	H	9.02633507	11.76424577	0.47326969
C	3.57233207	7.87871160	-4.19402488	H	8.34470847	10.69962841	-0.81873901
C	2.05065514	8.18444224	-4.14748026	H	6.55219251	7.98217250	4.93157186
C	1.34535085	7.12605588	-3.29602363	H	5.33297612	10.23092092	3.72147098
C	1.59369367	5.72454615	-3.83716994	H	10.83008188	10.13468649	0.44577977
C	3.11055877	5.48784942	-4.05737017	H	5.70088201	11.82137065	0.29465213
C	3.29540742	4.23489191	-4.93107857	H	3.46345401	11.36832879	-0.66523799
O	1.68659252	9.48485420	-3.70384904	H	4.12228608	8.37939155	-0.37746546
O	-0.06842867	7.41058317	-3.26850535	H	3.91889122	10.03180609	-2.95764705
O	1.17487742	4.72275315	-2.91532163	H	6.37194038	8.77659790	-1.58124628
O	3.75910885	6.59328121	-4.72650682	H	6.21367892	10.70895218	-3.95453882
O	4.58177707	3.64437583	-4.88136837	H	6.32952025	8.91462223	-4.12481321
C	-0.22192930	4.49249291	-2.77474779	H	4.02025708	9.84114039	1.66667094
C	-0.66218030	4.82605978	-1.32338233	H	1.90255220	9.29502374	-0.20518182
C	-0.02850437	3.82149884	-0.35941752	H	8.43922088	10.12171903	-4.04556838
C	-0.38987989	2.39422333	-0.77498970	H	4.07194733	8.57251775	-4.90495583
C	0.03271928	2.15166245	-2.24547724	H	1.69174644	8.10713714	-5.19416700
C	-0.43047863	0.80556499	-2.84442364	H	1.74757388	7.16741341	-2.26694109
O	-0.30039774	6.11979945	-0.88353584	H	1.05460810	5.61426558	-4.80633394
O	-0.47642181	4.04211632	0.97657108	H	3.57474767	5.33470805	-3.06181379
O	0.29420258	1.51568262	0.11167288	H	3.11015790	4.52820527	-5.98408256
O	-0.55042108	3.16202472	-3.08855331	H	2.51644430	3.50133382	-4.62971369
O	0.33408254	-0.30443700	-2.43960634	H	1.81743378	9.50839431	-2.71792545
H	-1.45306563	0.45476614	0.52954526	H	-0.13633352	8.39011514	-3.33089485
H	-0.65665594	-0.21820954	2.80385656	H	4.73822102	3.31045262	-3.95757902
H	1.81877937	1.43321106	2.08685953	H	-0.78681478	5.11181878	-3.49606927
H	1.62300968	-1.58752119	2.50770332	H	-1.76873513	4.68695584	-1.28879944
H	2.07989293	-0.13832225	-0.16248245	H	1.07589712	3.93424817	-0.41946308
H	3.04051270	-2.43434833	0.00029558	H	-1.48949619	2.26055634	-0.68132225
H	1.64835226	-2.35898303	-1.14196042	H	1.14047559	2.19603066	-2.30232749
H	-0.46450515	2.56601358	2.20537520	H	-0.31915972	0.90283149	-3.94311752
H	2.52823077	0.31602461	4.11699594	H	-1.52151543	0.67796086	-2.63587008
H	0.39440362	-3.15986819	0.71871503	H	-0.43053627	6.74671858	-1.63978360
H	3.55220852	-2.46276355	2.82153183	H	-0.29088898	4.97870481	1.18747588
H	5.65197156	-1.94609510	4.02520667	H	0.10512829	-0.53900415	-1.51141132
H	5.48444175	0.82037979	2.71007142	C	4.01022225	5.94578006	4.30775286
H	7.38096811	-1.56260843	2.30791547	C	3.29477648	5.74463413	2.94169480
H	5.28901829	-0.29360181	0.45545210	H	2.45173033	6.46576131	2.86848706
H	7.22879735	-1.12434945	-0.83195144	C	5.20302194	4.95089000	4.38980347
H	5.79881406	-2.19872197	-1.04216650	H	5.73489157	5.10022747	5.35520547
H	4.84911212	0.03096589	5.19559333	C	6.19286275	5.18440282	3.23222648
H	7.72479609	-0.07432727	4.12962582	H	6.64541769	6.18965767	3.30145352
H	6.84070440	-3.51134355	0.65559502	H	7.02400702	4.44941829	3.29492401
H	9.10804938	-1.24054246	0.86474117	C	4.27576902	6.00242333	1.78475288
H	10.92945886	-0.53336235	2.35565848	H	3.75811700	5.87391068	0.80942231
H	9.03191459	1.69474876	3.26899038	H	4.65375358	7.04115297	1.82472235
H	11.71360613	1.92416989	1.81074876	C	5.47404108	5.01189380	1.86367314
H	8.89305257	2.43940914	0.68222906	C	4.91451721	3.56685196	1.80125057
H	10.81334692	3.67843789	-0.39235787	H	5.74924426	2.83682044	1.86580434
H	11.65026216	2.10527613	-0.65771965	H	4.38232822	3.40217087	0.83929659
H	9.84969432	-0.71943592	4.41174433	C	2.73282619	4.29762441	2.88227717
H	10.86861449	2.20442055	4.60000443	H	2.20778919	4.14782947	1.91431816
H	9.63269325	1.54887922	-1.85236245	C	4.64455758	3.50452891	4.33399330
H	12.51851784	3.68249030	2.77884735	H	5.48898477	2.78638622	4.40427329
H	12.17592138	5.52862325	4.41969637	C	3.93441553	3.31643071	2.96617819
H	9.22313726	5.21844996	3.64265120	H	3.56399497	2.27586785	2.90576770
H	11.20018471	7.53578252	3.22290583	C	1.74446416	4.05515849	4.04201140
H	9.88867297	5.65582494	1.17790002	H	1.32186308	3.03390378	3.98702008
H	10.35861546	7.84548469	0.16742617	H	0.89578237	4.76836667	3.95833130
H	11.57532843	6.65325617	-0.37343427	C	3.64756886	3.25489470	5.48518029
H	10.53960432	4.30916387	5.79710721	H	4.16630939	3.36448665	6.46205991
H	8.95990282	6.89308074	5.19103424	H	3.25764735	2.21902576	5.42055887

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C 3.02544571 5.69823896 5.47040615
H 2.18970624 6.42879328 5.41646611
H 3.54231495 5.85706922 6.44177674
C 2.47310329 4.25662078 5.39012557
H 1.76522014 4.07814168 6.22473316
H 4.39503689 6.98802535 4.35154533
C 6.46124113 5.38767450 0.73981744
O 6.89984893 6.53637587 0.62958986
N 6.83304037 4.37787109 -0.11001792
H 6.31825940 3.50019577 -0.08225816
C 7.52169969 4.62583775 -1.35892125
H 7.83374202 5.68613734 -1.38638849
H 8.42242293 3.98419074 -1.43373138
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H 6.12292143 4.57833090 -4.46304383
C 7.85831416 5.71384222 -4.17421362
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10c_beta-CD_P:

C	1.40341431	-5.65796530	2.31570027	C	-2.81824652	-2.85881327	4.02535151
C	2.82441613	-5.85956129	2.89692006	C	-1.94351447	-3.51126070	5.11758109
O	2.82709144	-5.78720682	4.30530727	O	-1.97568778	-2.79322122	6.33633814
C	3.81769782	-4.86290520	2.25872545	C	-0.50133377	-3.68919077	4.61125142
O	5.16243879	-5.15087292	2.60803053	O	0.27621391	-4.44031480	5.53189356
C	3.68326165	-4.83606023	0.72912318	C	-0.47236804	-4.38068580	3.24615607
O	4.54739957	-3.80891118	0.26416181	O	0.89432261	-4.45193463	2.85388405
C	2.20795221	-4.52979240	0.38990160	C	-1.33743475	-3.54423394	2.27036458
O	1.41584521	-5.62096237	0.90362867	O	-2.68634915	-3.53324874	2.79464930
C	1.84421870	-4.29135030	-1.08533980	C	-1.40641275	-4.02164487	0.81051916
O	1.06576702	-3.10002985	-1.21737451	O	-1.40567886	-2.93323171	-0.11322390
C	5.41530078	-4.02803930	-0.82892299	H	0.75283021	-6.51126339	2.59388903
C	6.76540862	-3.37282156	-0.44202971	H	3.15770407	-6.87953299	2.61687007
O	7.25802947	-3.93881793	0.74958930	H	2.16517010	-5.11348416	4.58434599
C	6.55767618	-1.84740826	-0.38170232	H	3.54419238	-3.85045172	2.61304262
O	7.78325494	-1.18640587	-0.12971747	H	5.29945812	-4.79981783	3.51660225
C	5.89309861	-1.34623107	-1.67928922	H	3.97370113	-5.81886988	0.30018027
O	5.67284356	0.06200236	-1.50176212	H	1.93337174	-3.59704588	0.92141248
C	4.56807714	-2.09130378	-1.92842145	H	1.26539048	-5.16909378	-1.44560322
O	4.87598334	-3.49783483	-2.02283476	H	2.76316440	-4.20862121	-1.69492097
C	3.77524967	-1.68577323	-3.18609073	H	1.50782087	-2.47288816	-1.86598973
O	2.38964487	-1.50227986	-2.90144027	H	5.55713526	-5.11224737	-1.01010332
C	6.12320312	0.94142913	-2.49313570	H	7.50410045	-3.59088148	-1.23979819
C	6.69000544	2.21086192	-1.81821235	H	6.49602583	-4.09434038	1.35864101
O	7.63588049	1.82198625	-0.83431186	H	5.83278485	-1.66203513	0.43287727
C	5.56610237	3.06950171	-1.23448264	H	7.62868655	-0.22141748	-0.25075766
O	6.13433332	4.29140282	-0.78671390	H	6.58145469	-1.51835779	-2.53385332
C	4.48028111	3.30262958	-2.29475776	H	3.91410571	-1.91208347	-1.05461119
O	3.48259045	4.10508532	-1.66464120	H	3.89748238	-2.49679533	-3.93573289
C	3.96015128	1.94288865	-2.79720889	H	4.19604472	-0.75656345	-3.61281486
O	5.09456779	1.28828438	-3.40996154	H	2.11388178	-0.55751659	-3.08113395
C	2.79474602	1.98131229	-3.80902352	H	6.91332841	0.46882136	-3.11099988
O	1.75881890	1.06788424	-3.46592494	H	7.17979811	2.81075356	-2.61889299
C	2.95776178	5.21264342	-2.34720691	H	7.87509482	2.62826678	-0.33468734
C	2.84832001	6.39301735	-1.35001742	H	5.10184672	2.51108560	-0.38878382
O	4.06669798	6.62980868	-0.63489580	H	5.39012545	4.85391064	-0.47392213
C	1.76194884	6.12326789	-0.30784261	H	4.92412522	3.85313858	-3.15121659
O	1.50097441	7.28052164	0.47977189	H	3.61360385	1.35166990	-1.92827842
C	0.45149886	5.69473578	-0.98179988	H	3.20575069	1.70899659	-4.80401961
O	-0.43079033	5.35725176	0.07682947	H	2.38229931	3.00571906	-3.87442833
C	0.72448216	4.50101014	-1.92820441	H	0.94172349	1.55541959	-3.15412644
O	1.69173831	4.94275873	-2.91111369	H	3.60942692	5.49437771	-3.20231521
C	-0.49317138	3.90469570	-2.65841006	H	2.54931260	7.29477123	-1.92614737
O	-0.44915580	2.48021415	-2.68318188	H	4.70332235	7.07036125	-1.23042023
C	-1.76875582	5.81671570	0.06279878	H	2.09873201	5.27941658	0.33257126
C	-2.10207920	6.24115214	1.50770427	H	2.35311585	7.54874416	0.87821037
O	-1.19885220	7.20618439	2.01301681	H	0.04980281	6.54845428	-1.57022111
C	-2.16338268	4.99872237	2.41301015	H	1.16712039	3.68619506	-1.33194138
O	-2.63060805	5.33692435	3.71297434	H	-1.42542230	4.24201669	-2.16799475
C	-3.08884617	3.93620534	1.81263675	H	-0.48958789	4.28872952	-3.70051844
O	-3.02833529	2.80360302	2.67005716	H	-1.15781269	2.10714783	-2.08219140
C	-2.60508358	3.60243414	0.38205331	H	-1.88105434	6.67505482	-0.63019275
O	-2.65253272	4.82145250	-0.39674974	H	-3.10777629	6.70721073	1.50382350
C	-3.38864680	2.51568351	-0.37396642	H	-0.30086776	6.99936635	1.66095634
O	-2.51216763	1.62359646	-1.05739006	H	-1.14045206	4.56224872	2.46707166
C	-4.22773445	2.19841176	3.11353186	H	-2.11032177	6.11885003	3.99314365
C	-4.01493317	1.82070124	4.59388154	H	-4.12389040	4.33689870	1.76761183
O	-3.62479826	2.92331368	5.38966387	H	-1.55713911	3.25599615	0.45523403
C	-2.99701681	0.67029960	4.69310219	H	-4.05723956	3.02381950	-1.10238670
O	-2.87231327	0.21049843	6.03269887	H	-4.02080265	1.95092708	0.33654021
C	-3.41757833	-0.49278898	3.78952695	H	-2.65145715	0.69856221	-0.69456196
O	-2.42498161	-1.50428448	3.92467235	H	-5.07969838	2.90074545	3.01273722
C	-3.53730959	0.04311066	2.34063884	H	-4.98150785	1.45463789	4.99488363
O	-4.56005163	1.06910983	2.33908645	H	-3.07058090	3.52458865	4.83838241
C	-3.87769765	-0.97362731	1.23335775	H	-2.02096398	1.05325297	4.32567937
O	-3.07734514	-0.78961931	0.06680455	H	-2.77742442	1.01584946	6.58325981
C	-2.56929571	0.50136350	2.07461045	H	-4.40498402	-0.87750497	4.12401415

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C	-2.80244883	3.95916297	0.01646866	H	0.05994684	6.30241822	2.24054543
O	-2.46304201	5.28961639	-0.42802452	H	-1.38445164	3.99039569	2.32627835
C	-3.76428675	3.37434954	-1.00374887	H	-2.10811078	5.34603664	4.15299871
O	-3.05987694	3.12613486	-2.21737694	H	-4.25807994	4.67001142	1.48264527
C	-4.98106840	2.31676811	2.18795870	H	-1.88660547	3.33935759	0.02996902
C	-5.09173597	1.80582319	3.64111900	H	-4.58841297	4.10279672	-1.16425256
O	-4.79461685	2.82482040	4.56132793	H	-4.20536021	2.44180779	-0.59106747
C	-4.22651945	0.53965010	3.80397050	H	-3.71342904	3.23859239	-2.94364047
O	-4.54011607	-0.06905775	5.04479168	H	-5.67850724	3.16437393	2.03508306
C	-4.45931236	-0.45746366	2.64495564	H	-6.14680873	1.51165238	3.81353365
O	-3.40787563	-1.44268033	2.68337222	H	-3.96870925	3.27909222	4.27391223
C	-4.47960169	0.18441689	1.24456333	H	-3.16099569	0.86523209	3.75642683
O	-5.35083327	1.33011446	1.25564304	H	-3.81040635	-0.67859951	5.28942232
C	-4.98670115	-0.73826230	0.11470463	H	-5.44043105	-0.94589162	2.82121247
O	-3.94205985	-1.47356470	-0.47750224	H	-3.45520196	0.51152350	0.98516229
C	-3.64631893	-2.68269375	3.30852714	H	-5.43706468	-0.06868616	-0.65012268
C	-2.47960974	-2.95446255	4.29598716	H	-5.79930933	-1.39791895	0.49231359
O	-2.17313669	-1.80455794	5.10003048	H	-4.02708042	-2.44516889	-0.29709668
C	-1.19842042	-3.41671249	3.59009828	H	-4.60592712	-2.66420353	3.85977646
O	-0.27087904	-3.93575734	4.54364456	H	-2.79564462	-3.74478942	5.00098756
C	-1.43111422	-4.44712322	2.48418176	H	-1.91311683	-1.10094494	4.46585111
O	-0.20104814	-4.55139681	1.77093578	H	-0.75330966	-2.54103619	3.08343100
C	-2.57174201	-3.92004775	1.57812531	H	-0.13636148	-3.24754719	5.22562647
O	-3.75349233	-3.73868951	2.37982318	H	-1.72255017	-5.42231605	2.92823929
C	-2.91712088	-4.83300293	0.40334166	H	-2.26735785	-2.94220556	1.16367160
O	-3.88877445	-4.20011869	-0.42541150	H	-3.32218576	-5.79311173	0.79560014
H	-0.36649835	-6.63043460	1.71448422	H	-1.97654063	-5.04781899	-0.14732752
H	2.02167560	-7.05232969	2.11110389	H	-3.63563901	-4.24510825	-1.37705707
H	0.94655104	-5.12114503	3.92274861	C	1.06041361	-0.91135632	1.87951134
H	2.35384113	-4.00434699	2.01330163	C	-0.37840710	-0.40380390	1.63161816
H	3.68956345	-5.40816723	3.47936243	H	-1.07324089	-0.82998324	2.37872118
H	3.37828574	-6.22027988	0.15194264	C	2.00309881	-0.31544053	0.78719133
H	1.29129557	-3.97737156	-0.20273995	C	1.50368341	-0.72925341	-0.61531088
H	1.20049033	-6.18986392	-2.14470266	H	1.55058048	-1.83310471	-0.70443954
H	2.73664931	-5.26965998	-2.27234199	H	2.16720560	-0.31791723	-1.39643799
H	1.61923318	-3.51370812	-2.98574133	C	-0.84440798	-0.85502440	0.24232562
H	4.97960163	-5.61595178	-1.16913139	H	-1.90298682	-0.60430943	0.06367495
H	7.06856930	-4.37384621	-1.17169289	H	-0.76863720	-1.95823452	0.18394975
H	5.72942562	-4.46507164	1.32431139	C	0.05729951	-0.22864318	-0.85175015
H	5.64419823	-2.10046261	0.27437321	C	0.03354324	1.30311200	-0.70437515
H	7.62813606	-1.03043111	-0.38902854	H	0.67792997	1.73780645	-1.48685029
H	6.53741319	-2.11710382	-2.65418521	H	-0.99246640	1.66949893	-0.89758994
H	3.68734525	-2.25371943	-1.50017580	C	-0.40764034	1.13286697	1.78078470
H	4.30125557	-2.83039156	-4.39294418	H	-1.44352515	1.49809173	1.63182900
H	4.27040011	-1.10555862	-3.88531010	C	1.95802460	1.23733993	0.93401965
H	2.15360383	-1.20600901	-3.65668067	H	2.62473588	1.68856860	0.16904915
H	6.85876397	-0.08267597	-3.29907555	C	0.51306062	1.73088919	0.69249563
H	7.28276973	2.22955868	-2.64359790	H	0.48173836	2.83553432	0.76787033
H	8.01958616	1.79614009	-0.37863418	C	0.07890766	1.52879440	3.18814221
H	5.27517491	1.76141467	-0.37742330	H	0.04061679	2.63136907	3.31227515
H	5.68013973	4.02746327	-0.07268272	H	-0.60037217	1.09519404	3.95571576
H	5.08781648	3.46112403	-2.93543623	C	2.46794329	1.63674279	2.34311685
H	3.66003018	0.92397317	-1.95266107	H	2.44055088	2.74496696	2.43141554
H	3.30255900	1.95380013	-4.76050100	C	1.57397986	-0.51971817	3.28542790
H	2.34164752	2.74280886	-3.46339477	H	0.89982037	-0.97013981	4.04869148
H	1.04351093	1.05151455	-3.68291620	C	1.51763750	1.02640301	3.40998674
H	4.18319796	5.27355460	-2.51115610	H	1.86849524	1.32425905	4.42040071
H	3.22823290	6.88533808	-0.95274198	C	-0.51362968	-0.61138745	-2.22946105
H	5.20032552	6.29887528	-0.09917405	C	-1.26089476	-2.49153356	-3.66355481
H	2.22390188	4.51196144	0.69870725	H	-1.00381790	-1.88303969	-4.55403000
H	2.79361321	6.50500002	1.81754615	H	-0.90148102	-3.52322848	-3.79662493
H	0.66857203	6.57224260	-0.97432521	C	-2.78941799	-2.51998892	-3.43575634
H	1.23411991	3.56975695	-1.33744017	C	-4.66490500	-0.84693962	-3.35404077
H	-1.09764292	4.58538718	-2.19051848	C	-5.74021481	-1.71548381	-3.06335472
H	-0.04978856	5.26342684	-3.48351983	C	-4.90014904	0.53996116	-3.42754353
H	-0.85766986	2.63647098	-3.06423116	C	-7.02854820	-1.18193707	-2.85877189
H	-1.28123731	6.89933166	-0.14284566	H	-5.56253534	-2.78933435	-2.98071722
H	-2.70653269	6.71101834	1.84704043	C	-6.19432021	1.06434711	-3.25224102

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H	-4.06098373	1.22194720	-3.59933112	C	-2.54062589	4.33365752	-3.00344637
C	-7.26791200	0.20105451	-2.96445056	C	-2.92295153	3.31691086	-1.90939383
H	-8.28238582	0.58359991	-2.81526305	C	-2.77095371	3.88091207	-0.49536634
O	-0.94376201	0.23576684	-3.04003890	O	-4.75071673	2.88256077	-5.69512495
O	-3.39627393	-3.54616831	-3.12653620	O	-2.52814687	4.65566251	-5.46625787
C	-8.19991636	-2.05617100	-2.52030029	O	-1.14828444	4.63293645	-2.94354409
C	-6.37818291	2.53621490	-3.39487870	O	-4.31581585	2.96391801	-2.07406872
O	-7.86188964	-3.37065724	-2.42573965	O	-3.41343643	5.13911337	-0.32303138
H	-8.68778031	-3.85199853	-2.19860854	C	-0.83017017	6.00681647	-3.09519622
O	-7.66787093	2.92802997	-3.28033974	C	0.48795975	6.08737552	-3.89233524
H	-7.67690025	3.90449438	-3.39322169	C	1.70166312	5.70915536	-3.02819352
O	-5.48263278	3.34642705	-3.60626388	C	1.65657444	6.46119781	-1.69047476
O	-9.33429071	-1.65597618	-2.34224285	C	0.30008730	6.19746383	-1.00239689
N	-0.59730304	-1.93894209	-2.48853845	C	0.07156972	6.87759801	0.34762547
H	-0.14294608	-2.63175994	-1.88851741	O	0.41657827	5.32156110	-5.09442279
N	-3.35122436	-1.27691444	-3.59262255	O	2.92100707	6.03347047	-3.68432014
H	-2.66038812	-0.52335015	-3.72063683	O	2.75190017	5.97908208	-0.92535916
H	1.07731632	-2.01804009	1.78244464	O	-0.75387294	6.66740907	-1.86507843
C	3.43996790	-0.81462789	1.02271362	O	-0.98304452	6.27846008	1.07563035
H	3.46678721	-1.91768468	0.91581122	C	3.40949516	6.85570243	-0.02776299
H	4.10616161	-0.39258544	0.24534905	C	4.91943319	6.74996000	-0.32808963
C	3.94024935	-0.40894032	2.42499177	C	5.46011136	5.38567280	0.13304898
H	4.97722479	-0.77781445	2.56585413	C	5.05422922	5.08765096	1.57866772
C	3.01441835	-1.03209596	3.49408297	C	3.52015768	5.19427204	1.69328035
H	3.36834932	-0.76263354	4.51190040	C	2.94048739	4.91859952	3.08180778
C	3.90938383	1.13053088	2.55538401	O	5.21437753	6.98216206	-1.69286034
H	4.27510412	1.43754322	3.55836755	O	6.88087113	5.35985432	0.03279271
H	4.58474979	1.59194438	1.80345255	O	5.50182851	3.77441592	1.88145497
H	3.04218371	-2.13969105	3.41315895	O	3.13075540	6.53354402	1.31487533
				O	1.55869367	4.61140397	3.04519263
				C	6.21851534	3.52411945	3.07751772
				C	7.56059593	2.88141336	2.67919531
				C	7.26486369	1.52631389	2.02460232
				C	6.42382478	0.64428451	2.94451288
				C	5.14666131	1.38661814	3.40318617
				C	4.37593672	0.69041079	4.54320777
				O	8.35734522	3.69178188	1.84199256
				O	8.48254213	0.84418620	1.72851619
				O	6.08962375	-0.54377047	2.22057020
				O	5.49731143	2.67833115	3.93979284
				O	3.80335250	-0.54405478	4.18534876
				C	6.62653235	-1.77786861	2.64316170
				C	7.26169969	-2.49962259	1.43770850
				C	6.15813934	-2.95060914	0.46465355
				C	5.18876827	-3.86147171	1.22072220
				C	4.55683554	-3.05471956	2.37773093
				C	3.60418144	-3.83777894	3.30601651
				O	8.24843005	-1.75578036	0.75998237
				O	6.73192791	-3.65261393	-0.62655690
				O	4.21388656	-4.36433664	0.31176802
				O	5.62395824	-2.58172755	3.24942816
				O	2.35085846	-4.11482412	2.72925592
				H	4.61803543	-6.29000184	0.99193698
				H	4.07081675	-7.38817288	-1.13316248
				H	3.35444535	-4.59468212	-2.16060294
				H	1.60778291	-7.05177106	-1.55347199
				H	1.67749187	-4.34256145	-0.10897966
				H	-0.55898451	-5.51393598	-0.11950043
				H	0.19320565	-5.42133621	1.51230548
				H	5.80984939	-5.14272885	-1.36715827
				H	2.55481769	-6.04930617	-3.95131571
				H	0.94000211	-7.62637918	1.02365220
				H	0.22363457	-7.18676713	-3.08200479
				H	-0.84007140	-6.38165307	-5.10849848
				H	-0.23294235	-3.51342918	-4.21346444
				H	-2.88629553	-5.03585447	-4.36155997
				H	-1.29809707	-4.08380187	-1.90617785
				H	-3.74434605	-3.97302565	-1.52487392

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H	-2.99094352	-5.32339041	-0.59779173	C	-0.66587021	-1.94350774	-0.04621995
H	1.18008361	-5.25789050	-5.97807853	H	-0.31074174	-2.97890693	0.14046022
H	-1.88076609	-3.36283268	-6.09768103	H	-1.49890129	-2.00382346	-0.77966621
H	-3.71636490	-6.66488606	-2.41521884	C	-0.00885641	-1.24187749	2.28444620
H	-4.62339448	-3.86328400	-4.14086327	H	-0.36633570	-0.80254537	3.23955115
H	-5.50546631	-2.00949481	-5.48848476	H	0.38100523	-2.25659489	2.50757640
H	-2.83289955	-0.58337517	-5.02431893	C	-1.17252747	-1.31280156	1.26975784
H	-5.61664529	0.12913352	-3.95436241	C	-1.68935827	0.11337221	0.97671342
H	-3.14988520	-0.98880194	-2.46893927	H	-2.53878938	0.06061164	0.26622923
H	-4.58305835	0.50142051	-1.06671766	H	-2.06653569	0.57861162	1.91195933
H	-6.03329881	-0.46801220	-1.51959783	C	0.63082642	1.06168915	1.40312870
H	-3.82285782	-2.03203114	-7.19336768	H	0.27097440	1.53544833	2.33946069
H	-4.25375655	1.10681787	-6.09296038	C	-0.02161262	0.34203473	-0.92214715
H	-4.87172268	-2.27534012	-0.53737762	H	-0.85824972	0.28471073	-1.65711648
H	-5.72796132	2.18662201	-3.29721733	C	-0.54476134	0.96602463	0.39592183
H	-4.92988921	4.36460262	-4.24145218	H	-0.90789500	1.99104035	0.17985750
H	-2.27862076	2.82479957	-4.49865120	C	1.76034425	1.92039387	0.80472600
H	-3.13681629	5.24860142	-2.81565133	H	1.37937079	2.94326970	0.60238389
H	-2.29189997	2.40919378	-2.00413346	H	2.58588043	2.02649555	1.53693084
H	-1.70405249	4.05113410	-0.27666981	C	1.12939005	1.17923066	-1.53302200
H	-3.14807932	3.12099462	0.22481315	H	0.75120933	2.20216160	-1.75622327
H	-4.47532483	3.49558675	-6.40434829	C	2.80277341	-0.15760294	-0.21426514
H	-1.57892845	4.92659969	-5.37828111	H	3.63404237	-0.10554757	0.52149897
H	-4.37401993	5.00344022	-0.43655509	C	2.27772443	1.27655985	-0.49397240
H	-1.62849443	6.52715543	-3.66045123	H	3.10165109	1.89082850	-0.91949230
H	0.62235175	7.13800198	-4.21279374	H	2.02490593	-2.02414087	0.60689655
H	1.65324407	4.61826194	-2.79897907	C	1.01102555	-1.73984475	-1.95399730
H	1.76887648	7.54837872	-1.89271826	H	1.34868210	-2.77079020	-1.72866729
H	0.20973352	5.10181465	-0.85108502	H	0.17649203	-1.81784517	-2.68371615
H	-0.09856196	7.96575794	0.16189017	C	2.16396575	-0.89835433	-2.55575763
H	0.97892887	6.76753215	0.96303580	C	3.31685908	-0.81267269	-1.50882501
H	0.36498077	4.36063542	-4.87810356	H	4.15353914	-0.22529885	-1.93851952
H	2.87305752	5.65705620	-4.58622455	C	1.63212352	0.53495308	-2.83520621
H	-1.80517043	6.29748376	0.53925272	H	2.44449570	1.14069210	-3.28000251
H	3.05981464	7.89776059	-0.17152253	H	0.81042877	0.48910056	-3.58155614
H	5.44371560	7.53492480	0.25167288	H	3.69168314	-1.83492498	-1.29370855
H	5.01031970	4.59632569	-0.51120657	C	2.77566074	-1.44931006	-3.85302731
H	5.53148583	5.83330969	2.25049835	O	3.41284353	-0.69856965	-4.61270005
H	3.06977018	4.46649091	0.99163106	N	2.64743321	-2.77984395	-4.13991583
H	3.16780791	5.79251453	3.73928949	H	2.03197743	-3.38655774	-3.59621467
H	3.44756029	4.03067772	3.50294363	C	3.26148577	-3.36292693	-5.33676771
H	4.55694936	6.48202086	-2.23178171	H	3.43278846	-4.43631658	-5.16798743
H	7.10557267	5.69981707	-0.85826240	H	4.23279182	-2.85714866	-5.50506807
H	1.06120325	5.37591175	2.69521559	C	2.34364968	-3.16024977	-6.56632534
H	6.38644700	4.46424892	3.64127413	O	1.79715438	-4.08198044	-7.16790162
H	8.14601230	2.70302059	3.60356010	N	2.13169890	-1.82379655	-6.83599229
H	6.68496380	1.70661585	1.09314620	H	2.70566203	-1.19247171	-6.25263292
H	7.03253721	0.39214981	3.84029692	C	0.93128739	-1.25901209	-7.30693725
H	4.48062651	1.50605068	2.52548215	C	0.01578758	-1.95420870	-8.12191190
H	3.54737109	1.36499881	4.83701032	C	0.61195569	0.04033220	-6.85946925
H	5.06351849	0.60564625	5.41994818	C	-1.22443833	-1.36416714	-8.43483950
H	7.78623571	4.10616431	1.14641186	H	0.24240805	-2.96213135	-8.47561292
H	9.07336086	1.51020952	1.31527874	C	-0.61688327	0.63519618	-7.19761507
H	4.51801626	-1.19919819	4.02939146	H	1.30590647	0.59037924	-6.21044992
H	7.38837308	-1.61967865	3.43233028	C	-1.55422250	-0.07173863	-7.97962209
H	7.74484660	-3.41953001	1.83209110	H	-2.53128957	0.36552083	-8.20082562
H	5.60840069	-2.05256491	0.10583726	C	-2.15839512	-2.17919199	-9.27201140
H	5.76713358	-4.70552171	1.65434175	O	-1.86233517	-3.16356175	-9.91210363
H	4.00647596	-2.18824796	1.95975406	O	-3.44978134	-1.70258452	-9.22453380
H	3.42277087	-3.19928801	4.19239020	H	-3.98259647	-2.30402772	-9.79118173
H	4.12779785	-4.75976899	3.65793354	C	-0.89733429	1.99679191	-6.64819685
H	8.19387945	-0.79384276	0.99460940	O	-0.20806077	2.53546615	-5.78414197
H	7.50886202	-3.12834043	-0.91473364	O	-1.98909788	2.57785979	-7.17718928
H	2.45262606	-4.86689708	2.10227108	H	-2.14961517	3.44483700	-6.69477449
C	1.65213859	-1.00027966	0.39084677	H	-2.00184047	-1.92739246	1.67481492
C	1.13100991	-0.37472697	1.70822897				
H	1.96590728	-0.33039134	2.43720264				
C	0.48627647	-1.10633336	-0.64489923				

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C	4.09280833	-5.80371486	0.35710213	C	6.84363348	1.55040420	2.58560027
C	4.31067147	-6.20292946	-1.12076235	C	6.02455024	0.60515423	3.46326363
C	3.11376549	-5.73003968	-1.96637241	C	4.74045869	1.29524533	3.99739832
C	1.80496120	-6.20052392	-1.30177395	C	4.10080288	0.51651379	5.16469582
C	1.68576502	-5.79102215	0.17345472	O	7.92608025	3.72362739	2.56848026
C	0.49206479	-6.43079608	0.88897705	O	8.11449141	0.96170927	2.26360225
O	5.56585352	-5.74708541	-1.55575370	O	5.59301755	-0.54588558	2.73330984
O	3.22445244	-6.25648243	-3.26661707	O	5.01332177	2.60506865	4.52552995
O	0.72152418	-5.63323931	-2.04620617	O	3.61220094	-0.75663998	4.80507782
O	2.85786293	-6.27049389	0.88121887	C	6.51605112	-1.62019728	2.58464348
O	0.53790621	-7.84648424	0.83603510	C	6.82879510	-1.87023877	1.08168733
C	-0.23546961	-6.47477673	-2.62836308	C	5.67332409	-2.57117450	0.35810171
C	-0.49505302	-5.98207301	-4.06960950	C	5.22463194	-3.79342335	1.15605581
C	-1.09913016	-4.57490485	-4.01510114	C	4.82963833	-3.32435212	2.57070443
C	-2.37281943	-4.61744699	-3.17666397	C	4.26634002	-4.40294825	3.51706136
C	-2.05476167	-5.16727752	-1.77124776	O	7.11817139	-0.69656528	0.35117680
C	-3.29920727	-5.33744430	-0.89906379	O	6.07565394	-2.97083051	-0.94879032
O	0.72648643	-6.01350601	-4.79263586	O	4.13425991	-4.39422914	0.46645126
O	-1.31481621	-4.09392784	-5.34996363	O	6.00775291	-2.77611196	3.20453395
O	-2.89675406	-3.29723287	-3.09782469	O	2.91860136	-4.71794987	3.25529168
O	-1.45524061	-6.46942056	-1.89637381	H	4.87577182	-6.27244597	0.98543502
O	-4.28447380	-6.15227435	-1.51590060	H	4.33944107	-7.31025894	-1.17734645
C	-4.30537476	-3.16093451	-3.16291776	H	3.11164361	-4.61257444	-1.96699881
C	-4.69404352	-2.52390626	-4.51287738	H	1.76661922	-7.30674664	-1.35241460
C	-4.24431873	-1.06782360	-4.58912306	H	1.62906618	-4.68491935	0.25408909
C	-4.66794173	-0.28564246	-3.33944351	H	-0.43919088	-6.12319962	0.38107824
C	-4.23116042	-1.02865926	-2.06900811	H	0.46981087	-6.04980047	1.93782076
C	-4.69624274	-0.40071434	-0.75850350	H	5.58841023	-4.76289225	-1.49632962
O	-4.09865881	-3.28809208	-5.56862398	H	2.41755052	-5.99680908	-3.76930767
O	-4.79530570	-0.51682790	-5.77383497	H	1.40799609	-8.10628166	1.19978242
O	-3.99569306	0.97097914	-3.43750488	H	0.10337680	-7.52867187	-2.63302144
O	-4.76713777	-2.36684239	-2.09451826	H	-1.23711617	-6.67064617	-4.53383508
O	-4.08869580	-1.01928529	0.36348446	H	-0.36885357	-3.91357309	-3.51403089
C	-4.66414603	2.17774209	-3.22821938	H	-3.10148197	-5.29656532	-3.66262829
C	-4.32139348	3.11012876	-4.41286277	H	-1.35234179	-4.46725801	-1.27049757
C	-2.82626541	3.43547588	-4.38412138	H	-3.75792153	-4.34481701	-0.73157557
C	-2.45392491	3.99857796	-3.00388814	H	-2.97977570	-5.74952742	0.08661757
C	-2.83536267	2.97838809	-1.91871272	H	0.58495820	-5.51551385	-5.62244954
C	-2.48343119	3.38897724	-0.49398122	H	-2.21996725	-3.68417360	-5.40424312
O	-4.69840917	2.47810390	-5.62810734	H	-3.84452707	-6.99796936	-1.73693523
O	-2.56582211	4.35224142	-5.44697659	H	-4.79810543	-4.14360638	-3.03581202
O	-1.05423222	4.28510135	-2.98009302	H	-5.80239465	-2.55781606	-4.60013470
O	-4.26334306	2.78307247	-2.00154043	H	-3.13431291	-1.05326326	-4.62020735
O	-2.92849241	4.69819209	-0.14403945	H	-5.76985854	-0.14351951	-3.34666835
C	-0.73452556	5.64810875	-3.23720271	H	-3.12472043	-1.07338161	-2.05984765
C	0.65847770	5.66081636	-3.90088829	H	-4.40443850	0.66579228	-0.74390502
C	1.78495172	5.43486393	-2.87994328	H	-5.81133101	-0.45733172	-0.71412391
C	1.58418069	6.27312348	-1.61119866	H	-4.22785295	-2.75811726	-6.38339548
C	0.16099924	6.03218862	-1.05991616	H	-4.55992313	0.44070849	-5.79653810
C	-0.21981383	6.76773220	0.24555205	H	-4.25629498	-1.97931810	0.28096141
O	0.72740623	4.70858728	-4.96660780	H	-5.76027917	2.03289598	-3.14892241
O	3.05569252	5.75348342	-3.43638867	H	-4.88704486	4.05902001	-4.27620911
O	2.59309587	5.83297149	-0.71470043	H	-2.26622052	2.48871483	-4.54259801
O	-0.78306286	6.42590371	-2.07548444	H	-3.02771485	4.92394776	-2.79925414
O	-0.78027781	5.90704248	1.22253394	H	-2.32503231	2.01631955	-2.11857769
C	3.13428902	6.72413080	0.24309315	H	-1.38686435	3.39814257	-0.38830752
C	4.66689607	6.61597901	0.12560792	H	-2.88203069	2.62072616	0.20516174
C	5.15338833	5.26852674	0.68004657	H	-4.26174594	2.98530312	-6.34382926
C	4.58055590	4.99365649	2.07582040	H	-1.59460054	4.40297691	-5.57564617
C	3.04066868	5.08392187	1.97887664	H	-3.90488244	4.71127377	-0.15817217
C	2.25249645	4.77784856	3.25444230	H	-1.47988483	6.08833794	-3.92573715
O	5.12047198	6.81072003	-1.20283150	H	0.81097156	6.65417166	-4.36285145
O	6.57932425	5.26472485	0.72814562	H	1.75846669	4.36780630	-2.56151751
O	4.98457928	3.68777448	2.46368141	H	1.71812197	7.34911265	-1.85764482
O	2.69235410	6.41803202	1.54059517	H	0.07392563	4.94618165	-0.86074306
O	0.94583656	4.31851786	2.98067591	H	-0.91745694	7.58967507	-0.03201525
C	5.70426246	3.47882532	3.66868512	H	0.66657173	7.21133655	0.72497509
C	7.07915605	2.87917351	3.31664656	H	0.50534326	3.84251395	-4.55994797

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H	3.12802536	5.26196974	-4.27907142	C	0.33229821	0.99952319	-3.22604477
H	-1.63291527	5.54175963	0.88052211	H	0.79369658	1.52728897	-4.09061866
H	2.81101118	7.76424287	0.03573933	H	-0.76370456	1.10833779	-3.32468209
H	5.11987376	7.41855929	0.74035415	H	2.48659782	-1.74889119	-3.22019271
H	4.78986566	4.45936174	0.00823681	C	0.06519327	-1.12851966	-4.54233508
H	4.95803353	5.75640394	2.79053671	O	-0.93391374	-0.69334282	-5.09331400
H	2.70830213	4.34946392	1.22307740	H	-0.18944518	-1.26467662	2.61936745
H	2.26505093	5.68864273	3.90225156	O	0.65646057	-2.28126307	-4.91241870
H	2.77215612	3.96342551	3.79556390	H	-0.01549993	-2.80670674	-5.44177371
H	4.52699418	6.29365513	-1.79742279				
H	6.88947705	5.59100312	-0.14243891				
H	0.45256608	4.97799589	2.43566535				
H	5.82245642	4.42992708	4.22676392				
H	7.60548978	2.66890512	4.26969960				
H	6.27333474	1.74523190	1.65394120				
H	6.65700119	0.29873223	4.32680472				
H	4.02417747	1.37007830	3.15534808				
H	3.24245719	1.10768869	5.54080370				
H	4.85691569	0.46361780	5.98704730				
H	7.40880231	4.15095161	1.83509696				
H	8.68575937	1.72636046	2.01943894				
H	4.28900197	-1.19500785	4.25128249				
H	7.45644153	-1.38258268	3.11906682				
H	7.69233010	-2.57799672	1.06770792				
H	4.81682364	-1.86770150	0.29180513				
H	6.07280100	-4.50626780	1.23171324				
H	4.05357659	-2.54073559	2.47575078				
H	4.31457299	-3.97271519	4.53788705				
H	4.93388451	-5.29894388	3.50076914				
H	7.68900605	-0.10981376	0.91214826				
H	6.49570557	-2.19266977	-1.36694665				
H	2.87271666	-5.30240510	2.46577307				
C	2.05872645	-0.76609222	-0.63659638				
C	2.52216035	-0.16633993	0.71616642				
H	3.62247261	-0.26666843	0.81247931				
C	0.50652330	-0.63509058	-0.74788472				
C	-0.17836390	-1.34863043	0.43834115				
H	0.07118929	-2.43288115	0.40245867				
H	-1.28169206	-1.25429957	0.34159621				
C	1.83192628	-0.90774772	1.87974955				
H	2.20278297	-0.53088274	2.85195753				
H	2.08139904	-1.98847031	1.84117802				
C	0.30103009	-0.73991071	1.77443865				
C	-0.05985969	0.76259508	1.81514838				
H	-1.16185141	0.89031447	1.74240881				
H	0.26683210	1.21722657	2.77246097				
C	2.16658402	1.34398511	0.73377362				
H	2.50732971	1.79542475	1.68675229				
C	0.16226703	0.88635229	-0.70399090				
H	-0.94188398	0.98138194	-0.78514557				
C	0.62656768	1.49042604	0.64301353				
H	0.37802918	2.57242803	0.68445681				
C	2.84669225	2.06218234	-0.44838655				
H	2.59996423	3.14328531	-0.43515831				
H	3.95057430	1.97169639	-0.35891848				
C	0.82848656	1.60050695	-1.90280355				
H	0.55496603	2.67419277	-1.86788802				
C	2.71893992	-0.05718911	-1.84756016				
H	3.82073699	-0.18084482	-1.77298121				
C	2.36861838	1.45279479	-1.77861821				
H	2.85325407	1.98017457	-2.63003595				
H	2.32413315	-1.84577072	-0.66230543				
C	0.03718906	-1.23403028	-2.08428043				
H	0.30731806	-2.30893015	-2.11528156				
H	-1.06604095	-1.16515842	-2.16139772				
C	0.69314185	-0.50119146	-3.29750143				
C	2.22869702	-0.67280693	-3.17882171				
H	2.72962537	-0.17524377	-4.03612123				