Supporting Information for

NMR ^{1}H-Shielding Constants of Hydrogen Bond Donor Reflect Manifestation of the Pauli Principle

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Contents

S1 Additional computational details

All our computations were carried out within the framework of the DFT theory.[1] Geometry optimizations have been performed in C_S symmetry using the ω-B97XD hybrid functional[2] with the 6-311++G(d,p)[3] basis set. This functional include empirical dispersion and correction on long-range interactions, and has shown to be adequate to reproduce the structural and energetic properties of biological hydrogen-bonded systems.[4,5] Isotropic 1H nuclear magnetic shielding constants parameters were calculated at the B3LYP[6,7]/cc-pVTZ[8,9]] level, using the GIAO approximation.[10–12] For hydrogen atoms, shielding constants results obtained with our selected approach has shown to be in excellent agreement with those values reached with the best ab initio methods using very much larger basis sets.[13]

Atomic charges were obtained using the BLYP functional[7,14] with dispersion corrections as developed by Grimme,[15,16] BLYP-D3(BJ) combined with the TZ2P basis sets (no Gaussian functions are involved)[17] using the Voronoi deformation density (VDD) method.[18–21]

All the geometry optimizations and NMR parameters evaluations were performed using the GAUSSIAN09 program package.[22] Calculations related to the charge redistribution were done with the Amsterdam Density Functional (ADF) program (2017.107) developed by Baerends, Ziegler, and others.[23]

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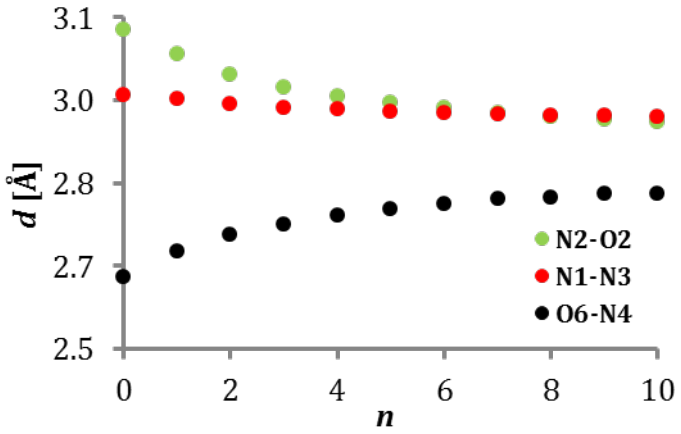
S2 Hydrogen bond donor-acceptor distances as a function of molecular structure

Table S1| Hydrogen bond lengths, *d*(X-Y), (in Å), for Z–$(C\equiv C)_n$– GC with a) Z = O^-, b) Z = OH, and c) Z = OH_2^+.[a]

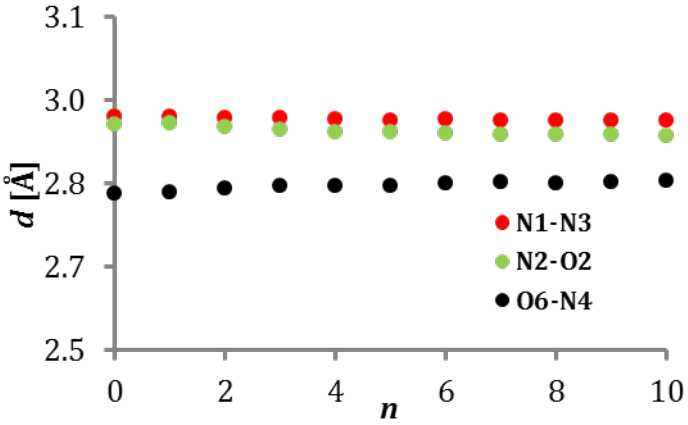
n	0	1	2	3	4	5	6	7	8	9	10	[(n=10)-(n=0)]
Z = O^-												
d(O6-N4)	2.63	2.68	2.71	2.73	2.74	2.75	2.76	2.77	2.77	2.78	2.78	0.15
d(N1-N3)	2.96	2.95	2.94	2.94	2.93	2.93	2.93	2.93	2.92	2.92	2.92	-0.04
d(N2-O2)	3.08	3.03	3.00	2.97	2.96	2.95	2.94	2.93	2.92	2.92	2.91	-0.17
Z = OH												
d(O6-N4)	2.78	2.78	2.79	2.79	2.80	2.79	2.80	2.80	2.80	2.80	2.80	0.02
d(N1-N3)	2.92	2.92	2.92	2.92	2.91	2.91	2.91	2.91	2.91	2.91	2.91	-0.01
d(N2-O2)	2.91	2.91	2.90	2.90	2.89	2.89	2.89	2.89	2.89	2.89	2.88	-0.02
Z = OH_2^+												
d(O6-N4)	2.89	2.87	2.86	2.85	2.84	2.84	2.83	2.83	2.82	2.82	2.82	-0.07
d(N1-N3)	2.88	2.89	2.89	2.90	2.90	2.90	2.90	2.90	2.90	2.91	2.91	0.03
d(N2-O2)	2.78	2.81	2.82	2.83	2.84	2.84	2.85	2.86	2.86	2.86	2.87	0.09

[a] Computed at ω-B97XD/6-311++G(d,p).

a) d(X-Y) / Z = O^-



b) d(X-Y) / Z = OH



c) d(X-Y) / Z = OH_2^+

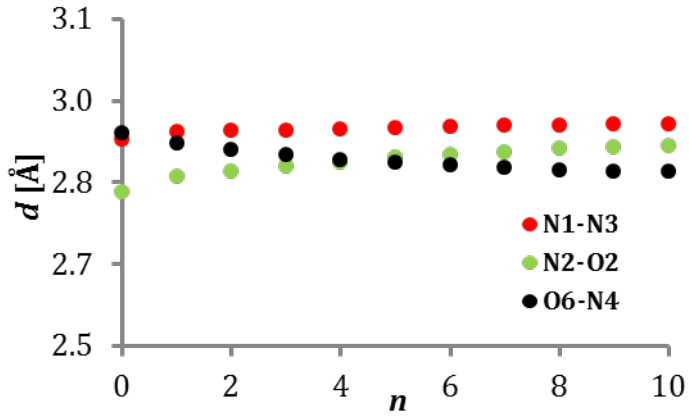


Figure S1| Hydrogen bond lengths, d(X-Y), for Z–$(C{\equiv}C)_n$–GC with a) Z = O^-, b) Z =OH, and c) OH_2^+.

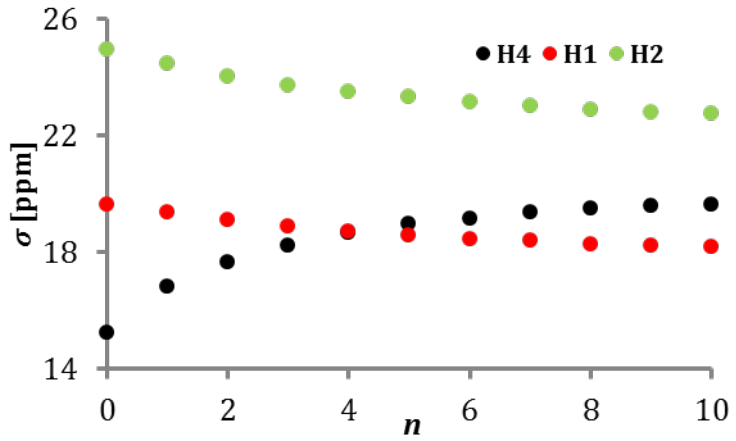
S3 ^{1}H-shielding values of H-bonded proton as a function of molecular structure

Table S2| ^{1}H-shielding, σ(H), values of H-bonded proton (in ppm) in Z–(C≡C)$_n$–GC with Z = O^-, OH, and OH_2^+.[a]

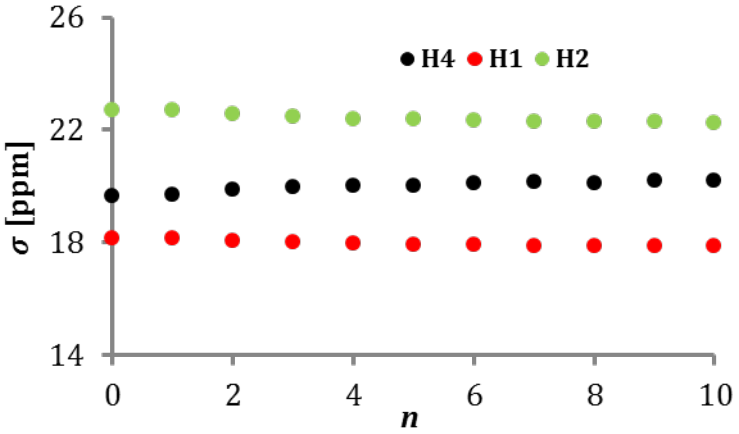
	Z=O$^-$			**Z=OH**			**Z=OH$_2^+$**		
n	σ(H4)	σ(H1)	σ(H2)	σ(H4)	σ(H1)	σ(H2)	σ(H4)	σ(H1)	σ(H2)
0	15.25	19.62	24.95	19.63	18.15	22.69	22.02	16.48	20.15
1	16.81	19.39	24.46	19.70	18.14	22.68	21.52	16.96	20.80
2	17.68	19.09	24.02	19.86	18.06	22.55	21.34	17.08	20.99
3	18.24	18.87	23.71	19.97	18.01	22.47	21.16	17.15	21.16
4	18.65	18.70	23.48	20.02	17.95	22.40	21.01	17.23	21.30
5	18.97	18.58	23.30	20.02	17.90	22.36	20.91	17.31	21.43
6	19.17	18.45	23.14	20.11	17.90	22.33	20.83	17.39	21.54
7	19.38	18.38	23.02	20.13	17.88	22.30	20.74	17.44	21.63
8	19.48	18.29	22.90	20.11	17.85	22.29	20.64	17.49	21.73
9	19.60	18.24	22.82	20.18	17.87	22.27	20.58	17.53	21.80
10	19.65	18.16	22.73	20.19	17.85	22.25	20.57	17.58	21.85

[a]Computed at B3LYP/cc-pVTZ

a) σ(H) / Z = O^-



b) σ(H) / Z = OH



c) σ(H) / Z = OH_2^+

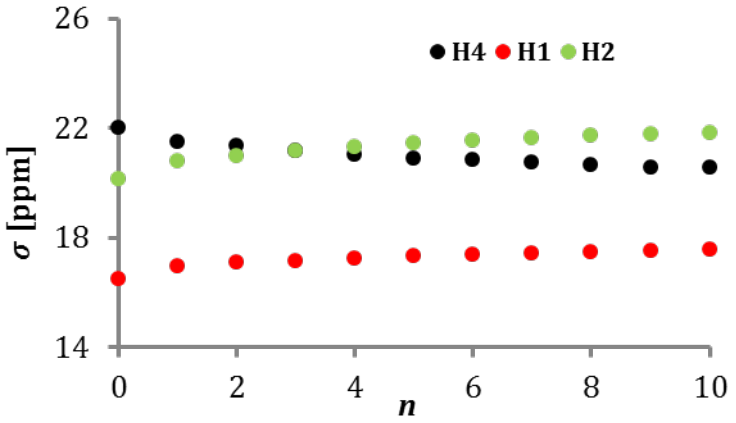


Figure S2| ^{1}H-shielding values, σ(H), of H-bonded proton as a function of molecular for Z–$(C\equiv C)_n$– GC with a) Z = O^-, b) Z = OH, and c) Z = OH_2^+.

S4 Voronoi deformation density (VDD) atomic charges analysis

Table S3| Voronoi deformation density (VDD) atomic charges, ΔQ(H), and contributions from Pauli repulsion, ΔQ_{Pauli}(H) , and bonding orbital interactions, ΔQ_{oi}(H), for H-bonded proton (in milli-electrons) in Z–(C≡C)$_n$–GC with Z = O^-, OH, and OH_2^+.[a]

Z=O^-

n	ΔQ(H4)	ΔQ(H1)	ΔQ(H2)	ΔQ_{Pauli}(H4)	ΔQ_{Pauli}(H1)	ΔQ_{Pauli}(H2)	ΔQ_{oi}(H4)	ΔQ_{oi}(H1)	ΔQ_{oi}(H2)
0	71.87	56.99	46.88	68.64	43.64	18.31	3.23	13.35	28.56
1	64.77	53.87	45.09	57.59	43.52	20.05	7.18	10.36	25.04
2	61.16	51.96	43.66	52.12	43.84	21.74	9.05	8.12	21.92
3	59.07	50.54	42.69	48.50	44.18	22.77	10.56	6.36	19.93
4	57.62	49.46	41.80	45.84	44.55	23.48	11.79	4.91	18.32
5	56.38	48.89	41.61	43.93	44.68	24.13	12.45	4.21	17.48
6	55.18	48.24	41.55	42.78	44.96	24.66	12.40	3.28	16.89
7	53.95	47.74	41.30	41.50	44.96	25.14	12.44	2.78	16.16
8	53.05	47.43	41.24	40.95	45.24	25.57	12.11	2.18	15.66
9	52.24	47.08	41.18	40.20	45.30	25.80	12.03	1.78	15.38
10	51.91	46.88	41.04	39.96	45.52	26.09	11.95	1.36	14.96

Z=OH

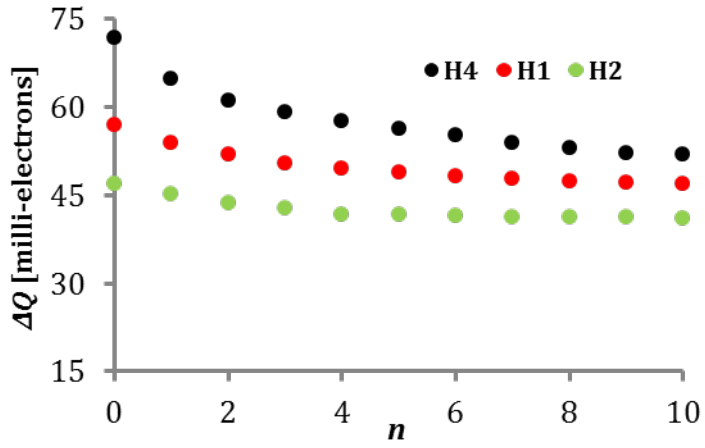
n	ΔQ(H4)	ΔQ(H1)	ΔQ(H2)	ΔQ_{Pauli}(H4)	ΔQ_{Pauli}(H1)	ΔQ_{Pauli}(H2)	ΔQ_{oi}(H4)	ΔQ_{oi}(H1)	ΔQ_{oi}(H2)
0	50.49	45.19	39.85	40.19	45.36	26.26	10.30	-0.17	13.58
1	50.24	45.23	39.67	39.51	45.23	26.27	10.74	0.00	13.40
2	49.25	44.89	39.93	38.56	45.30	26.61	10.69	-0.41	13.32
3	48.75	44.69	40.00	37.93	45.42	26.88	10.82	-0.73	13.12
4	48.37	44.55	40.06	37.66	45.65	27.16	10.71	-1.11	12.90
5	48.23	44.49	40.01	37.82	45.79	27.21	10.41	-1.30	12.80
6	47.76	44.36	40.10	37.11	45.68	27.29	10.65	-1.32	12.81
7	47.60	44.33	40.14	36.99	45.72	27.40	10.61	-1.39	12.74
8	47.59	44.28	40.10	37.17	45.83	27.39	10.43	-1.55	12.71
9	47.33	44.14	40.14	36.77	45.71	27.43	10.56	-1.57	12.70
10	47.23	44.10	40.21	36.70	45.76	27.59	10.53	-1.66	12.63

Z=OH_2^+

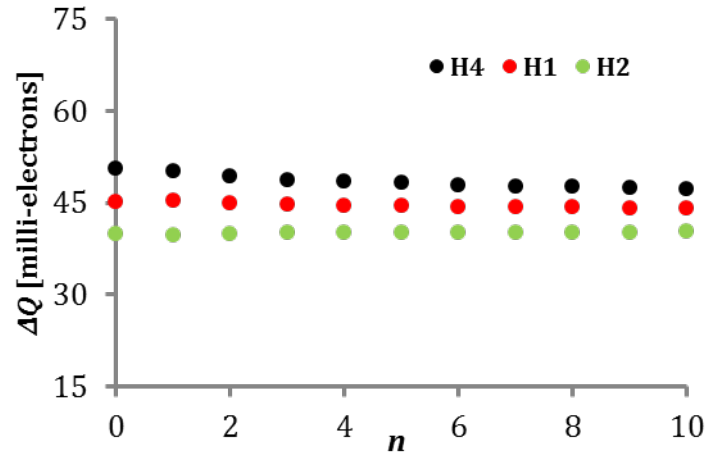
n	ΔQ(H4)	ΔQ(H1)	ΔQ(H2)	ΔQ_{Pauli}(H4)	ΔQ_{Pauli}(H1)	ΔQ_{Pauli}(H2)	ΔQ_{oi}(H4)	ΔQ_{oi}(H1)	ΔQ_{oi}(H2)
0	33.87	35.72	36.83	27.00	48.75	35.39	6.86	-13.03	1.44
1	37.32	38.48	38.25	29.28	47.36	33.04	8.04	-8.88	5.21
2	38.46	39.29	38.88	30.21	47.23	32.11	8.25	-7.94	6.77
3	39.91	40.10	39.37	31.24	47.19	31.40	8.67	-7.09	7.97
4	40.72	40.39	39.69	32.05	46.77	30.90	8.67	-6.38	8.79
5	41.31	40.81	39.80	32.61	46.57	30.38	8.70	-5.76	9.42
6	41.80	41.28	39.81	33.16	46.39	29.83	8.64	-5.10	9.98
7	42.38	41.43	40.08	33.61	46.21	29.58	8.77	-4.78	10.50
8	42.83	41.86	39.94	34.25	46.14	29.07	8.58	-4.29	10.87
9	43.39	41.42	38.92	34.43	46.13	28.87	8.95	-4.71	10.06
10	43.62	42.08	40.16	34.49	45.93	28.76	9.13	-3.86	11.39

[a] Computed at BLYP-D3(BJ)/TZ2P.

a) ΔQ(H) / Z = O^-



b) ΔQ(H) / Z = OH



c) ΔQ(H) / Z = OH_2^+

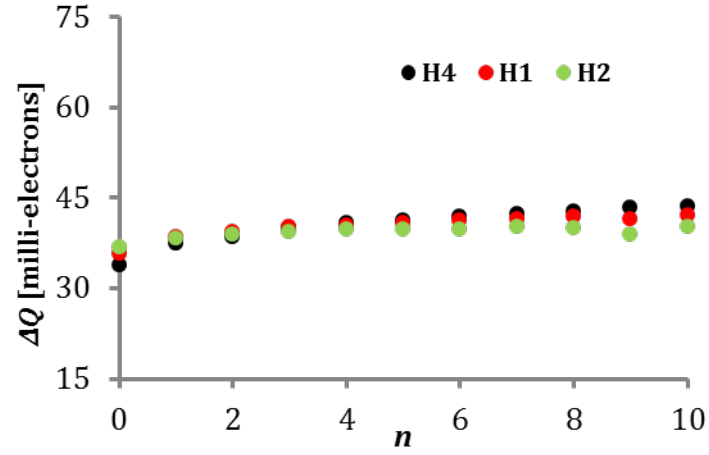
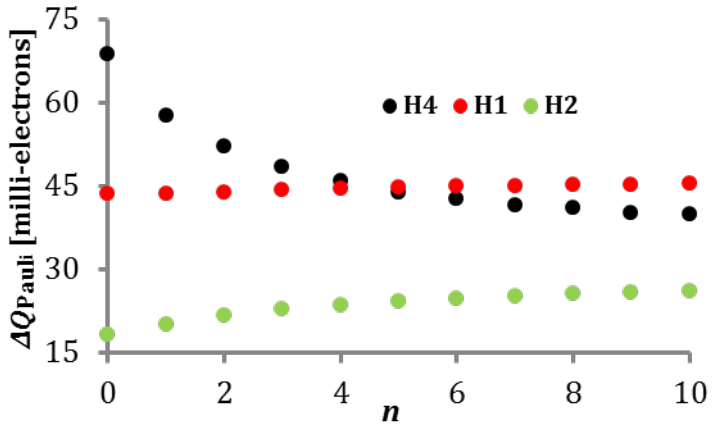
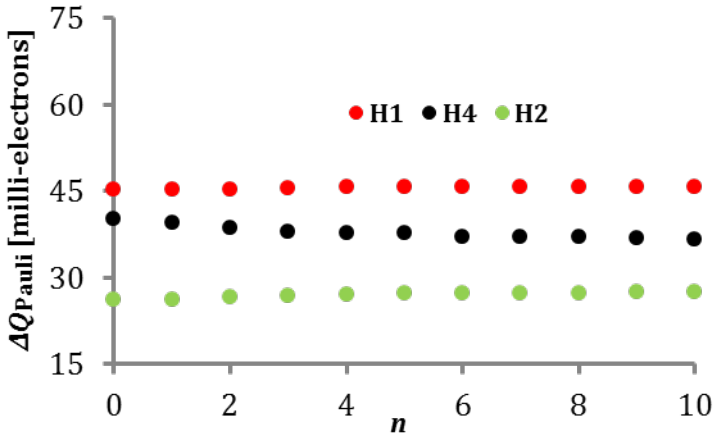


Figure S3| Voronoi deformation density (VDD) atomic charges, ΔQ(H) , (in milli-electrons) of H-bonded proton for Z–$(C\equiv C)_n$– GC with a) Z = O^-, b) Z = OH, and c) Z = OH_2^+.

a) $\Delta Q_{\text{Pauli}}(\text{H})$ / Z = O^-



b) $\Delta Q_{\text{Pauli}}(\text{H})$ / Z = OH



c) $\Delta Q_{\text{Pauli}}(\text{H})$ / Z = OH_2^+

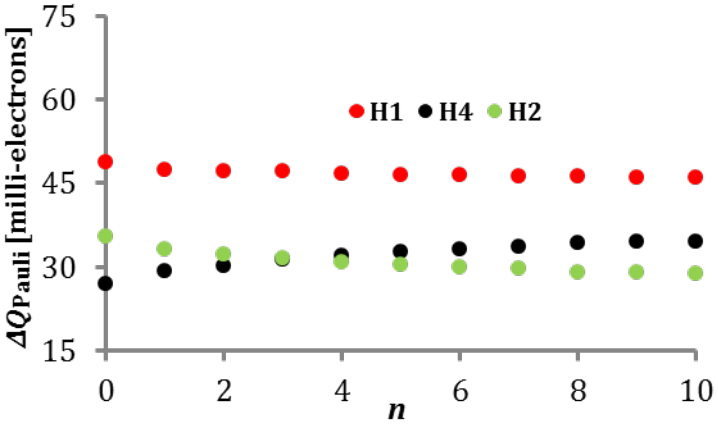
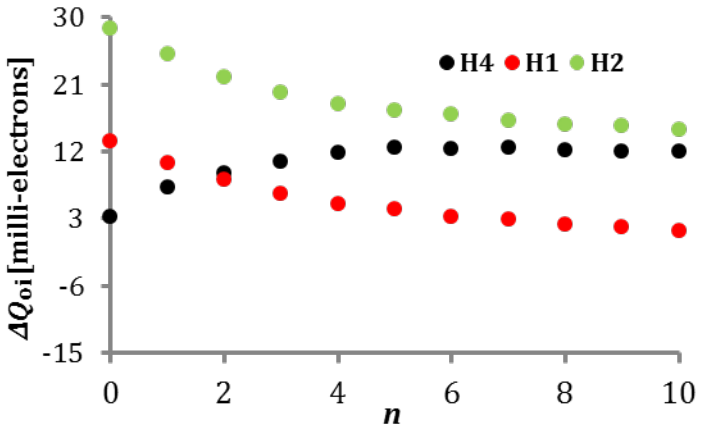
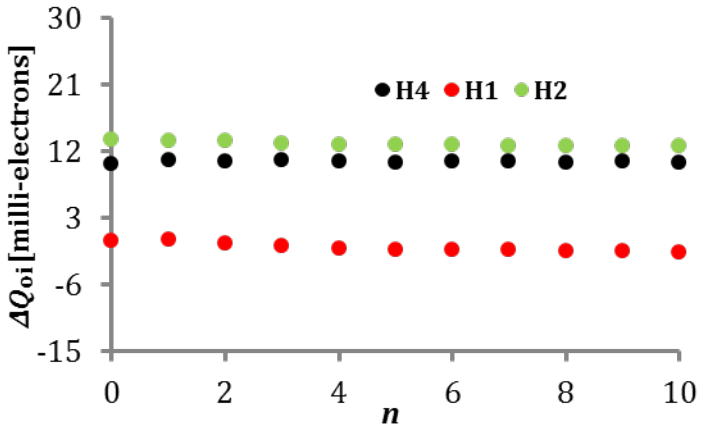


Figure S4| Voronoi deformation density (VDD) Pauli repulsion contribution to atomic charges, $\Delta Q_{\text{Pauli}}(\text{H})$, (in milli-electrons) of H-bonded proton for Z–$(C\equiv C)_n$– GC with a) Z = O^-, b) Z = OH, and c) Z = OH_2^+.

a) ΔQ_{oi}(H) / Z = O^-



b) ΔQ_{oi}(H) / Z = OH



c) ΔQ_{oi}(H) / Z = OH_2^+

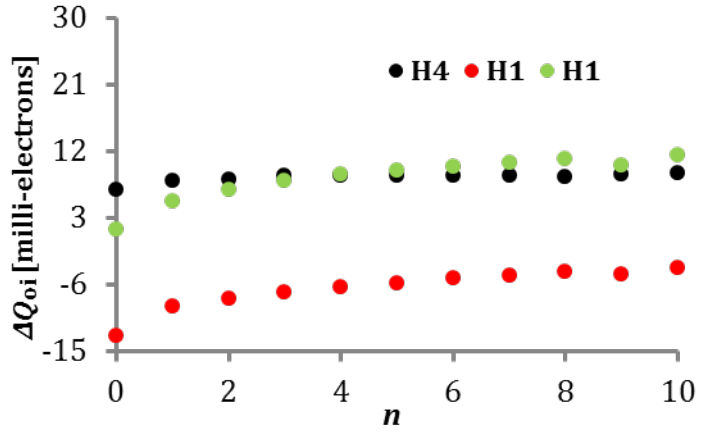
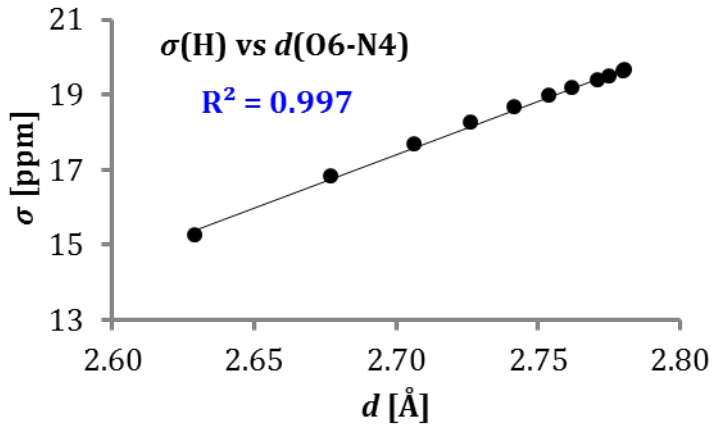


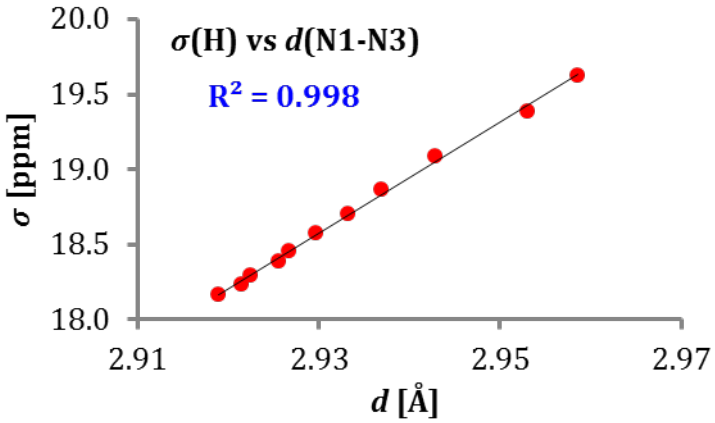
Figure S5| Voronoi deformation density (VDD) orbital interactions contribution to atomic charges, ΔQ_{oi}(H), (in milli-electrons) of H-bonded proton for Z–$(C\equiv C)_n$– GC with a) Z = O^-, b) Z = OH, and c) Z = OH_2^+.

S5 Linear regressions for VDD Pauli repulsion contribution to atomic charge, ^{1}H-shieldings and H-bond lengths

a) O6•••H4–N4



b) N1–H1•••N3



c) N2–H2•••O2

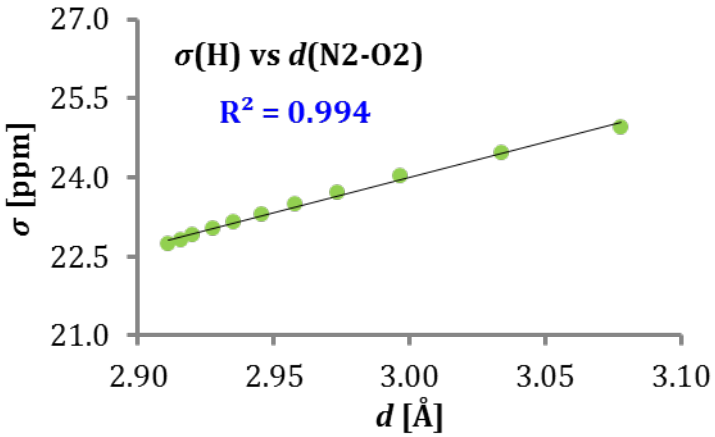
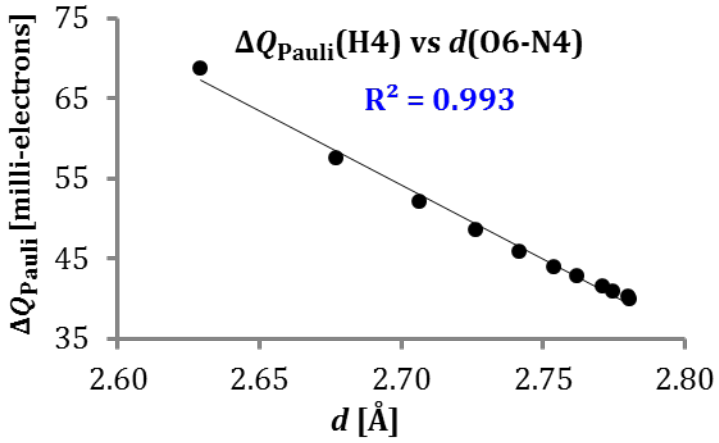
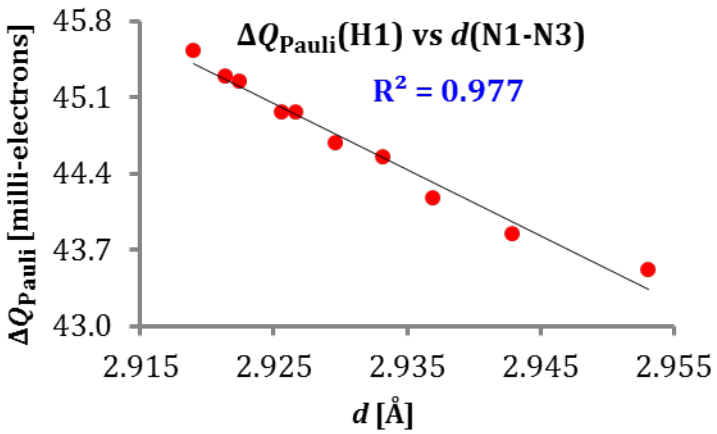


Figure S6| Relationship between ^{1}H-shielding values, σ(H), and H-bond length, d(X–Y), of H-bonded proton for O^{-}–$(C{\equiv}C)_n$– GC in a) O6•••H4–N4, b) N1–H1•••N3, and c) N2–H2•••O2.

a) O6•••H4–N4



b) N1–H1•••N3



c) N2–H2•••O2

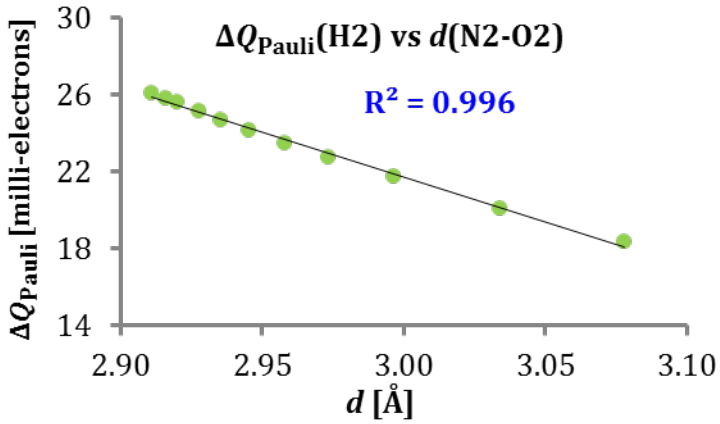
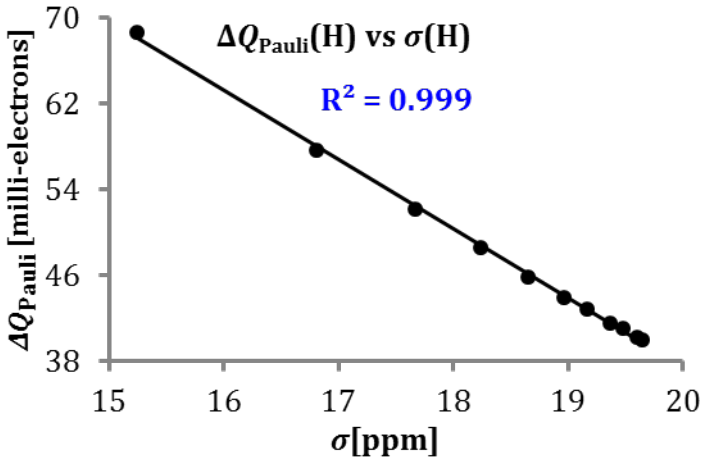
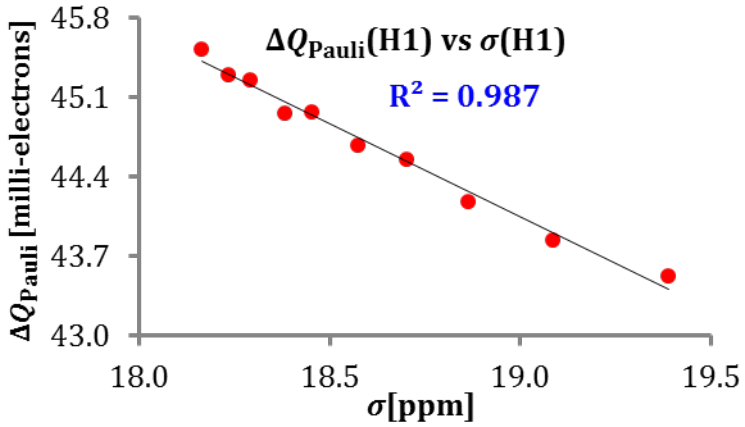


Figure S7| Relationship between VDD Pauli repulsion contribution to atomic charge, $\Delta Q_{\text{Pauli}}(\text{H})$, and H-bond length, d(X–Y), of H-bonded proton for O^{-}–$(C{\equiv}C)_n$– GC in a) O6•••H4–N4, b) N1–H1•••N3, and c) N2–H2•••O2.

a) O6•••H4–N4



b) N1–H1•••N3



c) N2–H2•••O2

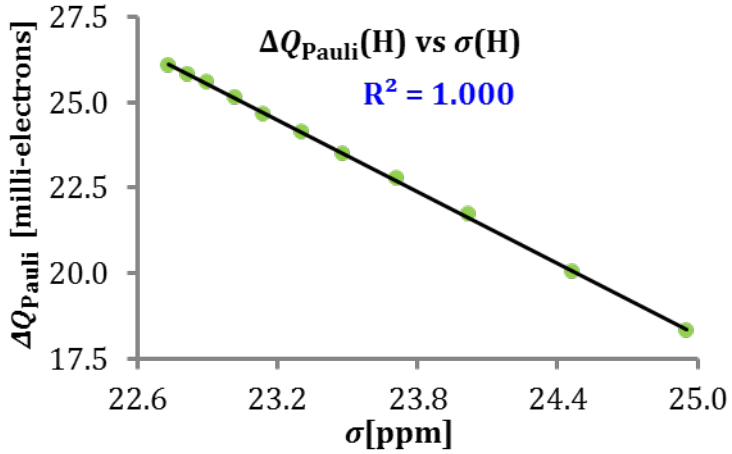
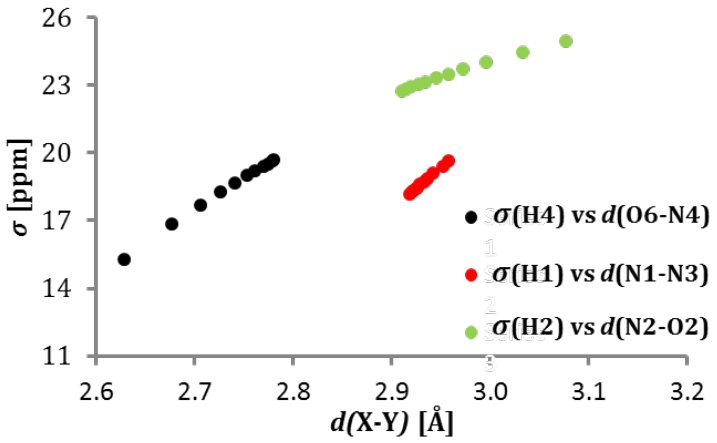


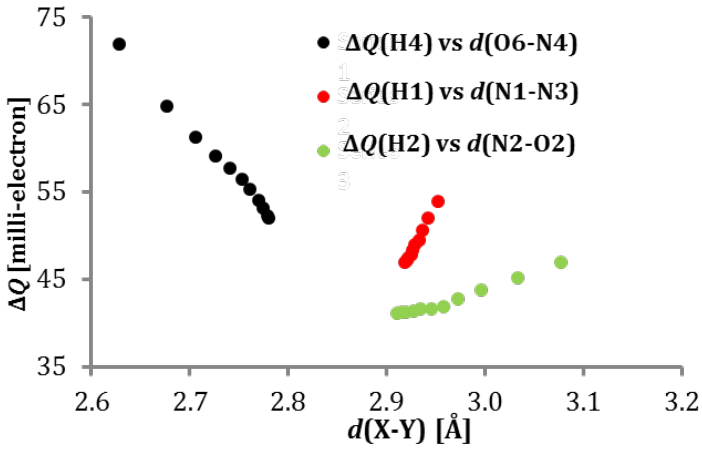
Figure S8| Relationship between VDD Pauli repulsion contribution to atomic charge, $\Delta Q_{\text{Pauli}}(\text{H})$, and ^{1}H-shielding values, σ(H), of H-bonded proton for O^{-}–$(C{\equiv}C)_n$– GC in a) O6•••H4–N4, b) N1–H1•••N3, and c) N2–H2•••O2.

S6 ^{1}H-shielding and VDD atomic charges of H-bonded proton as a function of donor-acceptor distance

a) σ(H) vs *d*(X-Y) / Z = O⁻



b) Δ*Q*(H) vs *d*(X-Y) / Z = O⁻



c) ΔQ_{Pauli}(H) vs *d*(X-Y) / Z = O⁻

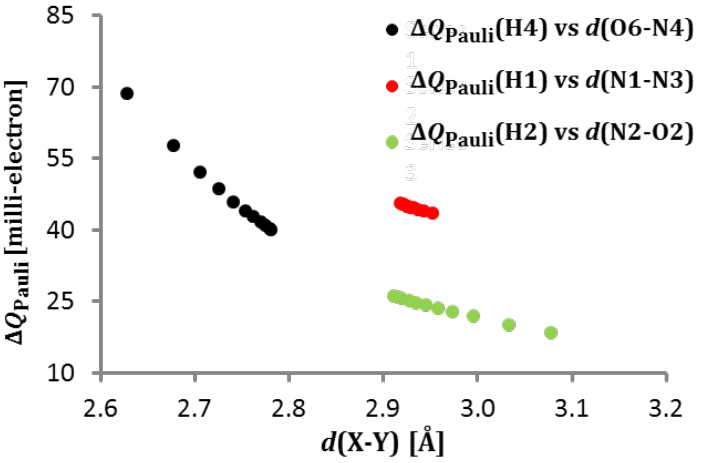


Figure S8| Relationship between a) σ(H) and *d*(X-Y), b) Δ*Q*(H) and *d*(X-Y), and c) ΔQ_{Pauli}(H) and *d*(X-Y) for O⁻-$(CC)_n$-GC systems, computed as described in **S1**.

S7 Cartesian coordinates for model systems Z–(C≡C)$_n$– GC

Table S5| Cartesian coordinates (in Å) of all O^--(CC)$_n$-GC systems, computed at ω-B97XD/6-311++G(d,p).

O^--GC

C	-0.59546900	1.78550200	0.00000000
C	1.42012200	2.72016600	0.00000000
C	2.14182500	1.51862200	0.00000000
C	1.38805600	0.33251900	0.00000000
C	3.66921600	3.06734900	0.00000000
N	-1.96245100	1.80000800	0.00000000
N	0.00000000	0.56605300	0.00000000
N	0.07789200	2.90792000	0.00000000
N	2.36312500	3.68753900	0.00000000
N	3.50315100	1.73618700	0.00000000
O	1.77392100	-0.86273100	0.00000000
O	4.68911600	3.76800300	0.00000000
H	-2.52053300	0.95479700	0.00000000
H	-2.40453500	2.69925300	0.00000000
H	-0.59105000	-0.26886100	0.00000000
H	2.20630800	4.67974200	0.00000000
C	-1.72046400	-4.32533800	0.00000000
C	-2.98072800	-1.83084400	0.00000000
C	-3.06502500	-4.25502800	0.00000000
C	-0.99391000	-3.07117100	0.00000000
N	0.32969800	-3.05962500	0.00000000
N	-1.63321200	-1.90096800	0.00000000
N	-3.68910000	-3.04900900	0.00000000
O	-3.62596200	-0.78978300	0.00000000
H	-1.20592700	-5.27584400	0.00000000
H	-4.69288800	-2.97201100	0.00000000
H	-3.70267000	-5.13096600	0.00000000
H	0.88267000	-2.14409900	0.00000000
H	0.82656000	-3.93331000	0.00000000

O^--CC-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.24069100
O	-0.00799500	0.00000000	2.44797500
C	-0.01361400	0.00000000	-1.38657900
N	-1.24624400	0.00000000	-2.07691300
N	0.98632700	0.00000000	-2.25771200
C	-0.99713400	0.00000000	-3.40587900
H	-2.14613900	0.00000000	-1.62920500
C	0.39518300	0.00000000	-3.50370800
N	-1.92081200	0.00000000	-4.39695500
C	0.95119200	0.00000000	-4.80181000
C	-1.38159200	0.00000000	-5.58985600
N	-0.03603700	0.00000000	-5.80209700
O	2.14579200	0.00000000	-5.15480400
N	-2.16916700	0.00000000	-6.69999600
H	0.31069900	0.00000000	-6.76611900
H	-1.79347900	0.00000000	-7.64203400
H	-3.16050700	0.00000000	-6.55067800
H	2.72917200	0.00000000	-6.66979100
N	3.14726500	0.00000000	-7.63780000
C	2.37737300	0.00000000	-8.71734200
H	4.14661700	0.00000000	-7.74110400
C	2.96732500	0.00000000	-10.03887400
N	1.05662300	0.00000000	-8.54556200
C	2.12077800	0.00000000	-11.08646000
H	4.03869000	0.00000000	-10.18038500
C	0.20853600	0.00000000	-9.59699100
N	0.77854100	0.00000000	-10.88350100
H	2.45563100	0.00000000	-12.11666600
O	-1.01252300	0.00000000	-9.50505100
H	0.12679000	0.00000000	-11.65116700

O^--(CC)$_2$ -GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.22758900
C	0.00000000	0.00000000	2.56476800
C	0.00000000	0.00000000	3.81083500
O	-0.00324300	0.00000000	5.01111000
C	-0.13349600	0.00000000	-1.39241300
N	-1.41207800	0.00000000	-1.96991900
N	0.79826500	0.00000000	-2.32457100
C	-1.26425900	0.00000000	-3.31642900
H	-2.27655800	0.00000000	-1.45601600
C	0.11421000	0.00000000	-3.52144900
N	-2.26037300	0.00000000	-4.23146600
C	0.57517400	0.00000000	-4.86117100
C	-1.81359400	0.00000000	-5.46333600
N	-0.48605800	0.00000000	-5.77945300
O	1.73677900	0.00000000	-5.29516700
N	-2.68201400	0.00000000	-6.50555100
H	-0.21306500	0.00000000	-6.76848600
H	-2.38028000	0.00000000	-7.47521000
H	-3.65907700	0.00000000	-6.27947100
H	2.22909600	0.00000000	-6.87977200
N	2.55984600	0.00000000	-7.87356800
C	1.69411600	0.00000000	-8.87944000
H	3.54622600	0.00000000	-8.06370600
C	2.16186700	0.00000000	-10.24765900
N	0.39522000	0.00000000	-8.58731000
C	1.22354200	0.00000000	-11.21398700
H	3.21611200	0.00000000	-10.48467700
C	-0.54476400	0.00000000	-9.55858300
N	-0.09458000	0.00000000	-10.88969400
H	1.46237000	0.00000000	-12.27044100
O	-1.75227800	0.00000000	-9.35418600
H	-0.81295500	0.00000000	-11.59566700

O^--(CC)$_3$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.22136900
C	0.00000000	0.00000000	2.56636500
C	0.00000000	0.00000000	3.80089400
C	0.00000000	0.00000000	5.12832600
C	0.00000000	0.00000000	6.37732900
O	-0.00075100	0.00000000	7.57299600
C	-0.13070800	0.00000000	-1.39903500
N	-1.40164300	0.00000000	-1.98028000
N	0.81097300	0.00000000	-2.31490100
C	-1.23945500	0.00000000	-3.32661200
H	-2.27323600	0.00000000	-1.47782800
C	0.13998600	0.00000000	-3.51785500
N	-2.22547300	0.00000000	-4.24998900
C	0.61874000	0.00000000	-4.85479500
C	-1.76530900	0.00000000	-5.47819200
N	-0.43321700	0.00000000	-5.78187300
O	1.78350500	0.00000000	-5.26962700
N	-2.62147500	0.00000000	-6.52641200
H	-0.14956800	0.00000000	-6.76925100
H	-2.30983800	0.00000000	-7.49391000
H	-3.60108300	0.00000000	-6.31046200
H	2.30800700	0.00000000	-6.86921200
N	2.64160600	0.00000000	-7.85752500
C	1.77692200	0.00000000	-8.86519200
H	3.62879300	0.00000000	-8.04303300
C	2.24660900	0.00000000	-10.23169300
N	0.47809100	0.00000000	-8.57381500
C	1.30936900	0.00000000	-11.19926600
H	3.30112600	0.00000000	-10.46720900
C	-0.46054300	0.00000000	-9.54714000

N	-0.00900200	0.00000000	-10.87649500
H	1.54926700	0.00000000	-12.25539200
O	-1.66819100	0.00000000	-9.34298600
H	-0.72632900	0.00000000	-11.58371900

O^--$(CC)_4$-GC

C	-3.03651207	-0.05519369	0.00000000
C	-4.25297748	-0.09865791	0.00000000
C	-5.60193830	-0.14685618	0.00000000
C	-6.82961456	-0.19072096	0.00000000
C	-8.16415559	-0.23840402	0.00000000
C	-9.40134477	-0.28260870	0.00000000
C	-10.72253932	-0.32981488	0.00000000
C	-11.97265025	-0.37448125	0.00000000
O	-13.16436218	-0.41667679	0.00000000
C	-1.63784407	0.11364135	0.00000000
N	-1.08937613	1.39555940	0.00000000
N	-0.70599898	-0.80880287	0.00000000
C	0.26097451	1.26143913	0.00000000
H	-1.60799513	2.25793849	0.00000000
C	0.48150508	-0.11313321	0.00000000
N	1.16197380	2.26599335	0.00000000
C	1.82995435	-0.56629566	0.00000000
C	2.40065454	1.83127512	0.00000000
N	2.73335919	0.50505301	0.00000000
O	2.26409112	-1.72135686	0.00000000
N	3.42822309	2.70860870	0.00000000
H	3.72738839	0.24180523	0.00000000
H	4.40301997	2.41811283	0.00000000
H	3.19073460	3.68345182	0.00000000
H	3.88905639	-2.22660390	0.00000000
N	4.88246393	-2.53463788	0.00000000
C	5.86627125	-1.64197038	0.00000000
H	5.09366133	-3.51659580	0.00000000
C	7.24452331	-2.07384402	0.00000000
N	5.53857509	-0.35192999	0.00000000
C	8.18586595	-1.11002443	0.00000000
H	7.50914653	-3.12138414	0.00000000
C	6.48629281	0.61315002	0.00000000
N	7.82676255	0.19878454	0.00000000
H	9.24816231	-1.32065623	0.00000000
O	6.24804469	1.81466576	0.00000000
H	8.51396635	0.93547493	0.00000000

O^--$(CC)_5$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.21444400
C	0.00000000	0.00000000	2.56759000
C	0.00000000	0.00000000	3.79153700
C	0.00000000	0.00000000	5.13231000
C	0.00000000	0.00000000	6.36412200
C	0.00000000	0.00000000	7.69438400
C	0.00000000	0.00000000	8.93441400
C	0.00000000	0.00000000	10.25281000
C	0.00000000	0.00000000	11.50502700
O	-0.00016300	0.00000000	12.69513600
C	-0.09594800	0.00000000	-1.40762400
N	-1.34330200	0.00000000	-2.02612900
N	0.87947100	0.00000000	-2.28180700
C	-1.13018100	0.00000000	-3.36682000
H	-2.23546800	0.00000000	-1.56043400
C	0.25487200	0.00000000	-3.50666600
N	-2.07926500	0.00000000	-4.32452500
C	0.78888200	0.00000000	-4.82697000
C	-1.57156600	0.00000000	-5.53619100
N	-0.22746800	0.00000000	-5.79081300
O	1.96682100	0.00000000	-5.18818000
N	-2.38612000	0.00000000	-6.61191400
H	0.09445600	0.00000000	-6.76810000
H	-2.03878600	0.00000000	-7.56829800
H	-3.37331100	0.00000000	-6.43210900
H	2.58042600	0.00000000	-6.79104100
N	2.94050500	0.00000000	-7.76443100
C	2.10092200	0.00000000	-8.79450900
H	3.93220400	0.00000000	-7.92314700
C	2.60647700	0.00000000	-10.14692400
N	0.79541500	0.00000000	-8.53609900
C	1.69483400	0.00000000	-11.13884300
H	3.66659800	0.00000000	-10.35479600
C	-0.11692000	0.00000000	-9.53524300
N	0.36870300	0.00000000	-10.85067100
H	1.96227000	0.00000000	-12.18811300
O	-1.32952300	0.00000000	-9.36146400
H	-0.33004600	0.00000000	-11.57642300

O^--$(CC)_6$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.21269100
C	0.00000000	0.00000000	2.56807400
C	0.00000000	0.00000000	3.78887600
C	0.00000000	0.00000000	5.13374600
C	0.00000000	0.00000000	6.36089100
C	0.00000000	0.00000000	7.69697400
C	0.00000000	0.00000000	8.93087500
C	0.00000000	0.00000000	10.25775800
C	0.00000000	0.00000000	11.49931000
C	0.00000000	0.00000000	12.81510900
C	0.00000000	0.00000000	14.06837800
O	-0.00015600	0.00000000	15.25678600
C	-0.08803800	0.00000000	-1.40938000
N	-1.32883900	0.00000000	-2.03862600
N	0.89692200	0.00000000	-2.27155200
C	-1.10062500	0.00000000	-3.37740500
H	-2.22712800	0.00000000	-1.58441000
C	0.28595600	0.00000000	-3.50203100
N	-2.03849700	0.00000000	-4.34482100
C	0.83577900	0.00000000	-4.81748300
C	-1.51709700	0.00000000	-5.55167700
N	-0.16956900	0.00000000	-5.79184700
O	2.01740600	0.00000000	-5.16241600
N	-2.31953500	0.00000000	-6.63476000
H	0.16337600	0.00000000	-6.76636400
H	-1.96198500	0.00000000	-7.58814600
H	-3.30881200	0.00000000	-6.46556700
H	2.65307700	0.00000000	-6.76649700
N	3.02148500	0.00000000	-7.73538900
C	2.18979100	0.00000000	-8.77221300
H	4.01471300	0.00000000	-7.88463900
C	2.70497400	0.00000000	-10.12053600
N	0.88239800	0.00000000	-8.52290400
C	1.80015600	0.00000000	-11.11896400
H	3.76660700	0.00000000	-10.32100100
C	-0.02279700	0.00000000	-9.52873400
N	0.47203900	0.00000000	-10.84020600
H	2.07507300	0.00000000	-12.16639300
O	-1.23667000	0.00000000	-9.36294300
H	-0.22142800	0.00000000	-11.57123100

O^--$(CC)_7$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.21150000
C	0.00000000	0.00000000	2.56835600
C	0.00000000	0.00000000	3.78687300
C	0.00000000	0.00000000	5.13483500
C	0.00000000	0.00000000	6.35838500
C	0.00000000	0.00000000	7.69921600
C	0.00000000	0.00000000	8.92814100
C	0.00000000	0.00000000	10.26126900
C	0.00000000	0.00000000	11.49653300
C	0.00000000	0.00000000	12.82107100
C	0.00000000	0.00000000	14.06367100
C	0.00000000	0.00000000	15.37758200
C	0.00000000	0.00000000	16.63160100

O	-0.00009200	0.00000000	17.81873100
C	-0.08517900	0.00000000	-1.41017800
N	-1.32242800	0.00000000	-2.04445800
N	0.90473000	0.00000000	-2.26605900
C	-1.08637000	0.00000000	-3.38212700
H	-2.22395400	0.00000000	-1.59650900
C	0.30098800	0.00000000	-3.49903600
N	-2.01821400	0.00000000	-4.35421300
C	0.85940600	0.00000000	-4.81211200
C	-1.48972100	0.00000000	-5.55874500
N	-0.14049900	0.00000000	-5.79161300
O	2.04250600	0.00000000	-5.14807500
N	-2.28586600	0.00000000	-6.64504200
H	0.19827200	0.00000000	-6.76461000
H	-1.92314500	0.00000000	-7.59687900
H	-3.27614000	0.00000000	-6.48121500
H	2.69363200	0.00000000	-6.75724200
N	3.06412900	0.00000000	-7.72394400
C	2.23435600	0.00000000	-8.76265900
H	4.05775400	0.00000000	-7.87043000
C	2.75238200	0.00000000	-10.10949900
N	0.92654400	0.00000000	-8.51565800
C	1.84963900	0.00000000	-11.10988400
H	3.81440200	0.00000000	-10.30773000
C	0.02361100	0.00000000	-9.52380200
N	0.52101200	0.00000000	-10.83386400
H	2.12673000	0.00000000	-12.15670300
O	-1.19063700	0.00000000	-9.36025800
H	-0.17090300	0.00000000	-11.56642800

O^--$(CC)_8$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.21073000
C	0.00000000	0.00000000	2.56847900
C	0.00000000	0.00000000	3.78540400
C	0.00000000	0.00000000	5.13555600
C	0.00000000	0.00000000	6.35647500
C	0.00000000	0.00000000	7.70097300
C	0.00000000	0.00000000	8.92605000
C	0.00000000	0.00000000	10.26434600
C	0.00000000	0.00000000	11.49448200
C	0.00000000	0.00000000	12.82554100
C	0.00000000	0.00000000	14.06180300
C	0.00000000	0.00000000	15.38462600
C	0.00000000	0.00000000	16.62802300
C	0.00000000	0.00000000	17.94052400
C	0.00000000	0.00000000	19.19511900
O	-0.00007300	0.00000000	20.38128100
C	-0.08316400	0.00000000	-1.41059000
N	-1.31772700	0.00000000	-2.04868700
N	0.91060500	0.00000000	-2.26174900
C	-1.07573600	0.00000000	-3.38550300
H	-2.22175300	0.00000000	-1.60565000
C	0.31237600	0.00000000	-3.49644300
N	-2.00293600	0.00000000	-4.36107300
C	0.87713100	0.00000000	-4.80788000
C	-1.46904300	0.00000000	-5.56386900
N	-0.11848300	0.00000000	-5.79112500
O	2.06151000	0.00000000	-5.13675200
N	-2.26025200	0.00000000	-6.65262600
H	0.22466400	0.00000000	-6.76310200
H	-1.89346700	0.00000000	-7.60333400
H	-3.25128900	0.00000000	-6.49295400
H	2.72329700	0.00000000	-6.74663400
N	3.09619800	0.00000000	-7.71163400
C	2.26815800	0.00000000	-8.75200900
H	4.09006200	0.00000000	-7.85639800
C	2.78863900	0.00000000	-10.09764300
N	0.95990100	0.00000000	-8.50735900
C	1.88771600	0.00000000	-11.09973300
H	3.85100500	0.00000000	-10.29393100
C	0.05891900	0.00000000	-9.51745400
N	0.55857800	0.00000000	-10.82618400
H	2.16673200	0.00000000	-12.14601400
O	-1.15565900	0.00000000	-9.35569900
H	-0.13196300	0.00000000	-11.56011000

O^--$(CC)_9$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.21023000
C	0.00000000	0.00000000	2.56845000
C	0.00000000	0.00000000	3.78428100
C	0.00000000	0.00000000	5.13588700
C	0.00000000	0.00000000	6.35490200
C	0.00000000	0.00000000	7.70208300
C	0.00000000	0.00000000	8.92425500
C	0.00000000	0.00000000	10.26662400
C	0.00000000	0.00000000	11.49269700
C	0.00000000	0.00000000	12.82922400
C	0.00000000	0.00000000	14.06021900
C	0.00000000	0.00000000	15.38976000
C	0.00000000	0.00000000	16.62675700
C	0.00000000	0.00000000	17.94829800
C	0.00000000	0.00000000	19.19229300
C	0.00000000	0.00000000	20.50372200
C	0.00000000	0.00000000	21.75875800
O	-0.00002700	0.00000000	22.94419000
C	-0.07822200	0.00000000	-1.41092600
N	-1.30947500	0.00000000	-2.05471200
N	0.92019000	0.00000000	-2.25645700
C	-1.06004800	0.00000000	-3.39021500
H	-2.21630400	0.00000000	-1.61733100
C	0.32882300	0.00000000	-3.49366100
N	-1.98154000	0.00000000	-4.37036600
C	0.90140400	0.00000000	-4.80251800
C	-1.44085000	0.00000000	-5.57066500
N	-0.08884400	0.00000000	-5.79083100
O	2.08735900	0.00000000	-5.12318900
N	-2.22608000	0.00000000	-6.66277500
H	0.25970500	0.00000000	-6.76130300
H	-1.85452100	0.00000000	-7.61197500
H	-3.21796300	0.00000000	-6.50794800
H	2.76213500	0.00000000	-6.73407300
N	3.13780800	0.00000000	-7.69720700
C	2.31308000	0.00000000	-8.74040700
H	4.13216200	0.00000000	-7.83857800
C	2.83830000	0.00000000	-10.08394500
N	1.00402900	0.00000000	-8.50012300
C	1.94095600	0.00000000	-11.08927700
H	3.90133100	0.00000000	-10.27653900
C	0.10677000	0.00000000	-9.51369000
N	0.61090800	0.00000000	-10.82037600
H	2.22366000	0.00000000	-12.13455200
O	-1.10841200	0.00000000	-9.35603000
H	-0.07700800	0.00000000	-11.55681800

O^--$(CC)_{10}$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.25537400
C	0.00000000	0.00000000	2.56599600
C	0.00000000	0.00000000	3.81045200
C	0.00000000	0.00000000	5.13101800
C	0.00000000	0.00000000	6.36857900
C	0.00000000	0.00000000	7.69698800
C	0.00000000	0.00000000	8.92862800
C	0.00000000	0.00000000	10.26387100
C	0.00000000	0.00000000	11.49065700
C	0.00000000	0.00000000	12.83157500
C	0.00000000	0.00000000	14.05455300
C	0.00000000	0.00000000	15.39999400
C	0.00000000	0.00000000	16.62003800
C	0.00000000	0.00000000	17.96911200
C	0.00000000	0.00000000	19.18679100
C	0.00000000	0.00000000	20.53933700

C	0.00000000	0.00000000	21.75443600	H	-1.82774100	0.00000000	31.94056100
C	0.00000000	0.00000000	23.11287900	H	-3.19525000	0.00000000	30.84094700
C	0.00000000	0.00000000	24.32280500	H	2.78816200	0.00000000	31.04500000
O	0.00001300	0.00000000	-1.18487900	N	3.16661800	0.00000000	32.00667500
C	-0.07567000	0.00000000	25.73380500	C	2.34478600	0.00000000	33.05223400
N	-1.30450400	0.00000000	26.38147400	H	4.16142400	0.00000000	32.14491600
N	0.92612100	0.00000000	26.57539800	C	2.87329500	0.00000000	34.39427500
C	-1.04994700	0.00000000	27.71607400	N	1.03505200	0.00000000	32.81524300
H	-2.21330000	0.00000000	25.94808300	C	1.97847700	0.00000000	35.40190200
C	0.33966000	0.00000000	27.81421000	H	3.93680600	0.00000000	34.58417600
N	-1.96736200	0.00000000	28.69929100	C	0.14042400	0.00000000	33.83119300
C	0.91751500	0.00000000	29.12129500	N	0.64773700	0.00000000	35.13635500
C	-1.42188900	0.00000000	29.89797300	H	2.26372000	0.00000000	36.44646800
N	-0.06892100	0.00000000	30.11308700	O	-1.07521500	0.00000000	33.67627000
O	2.10448200	0.00000000	29.43664200	H	-0.03822600	0.00000000	35.87467100
N	-2.20277900	0.00000000	30.99239200				
H	0.28356600	0.00000000	31.08255300				

Table S6| Cartesian coordinates (in Å) of all HO-(CC)$_n$-GC systems, computed at ω-B97XD/6-311++G(d,p).

HO-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.21128016
C	1.37751355	0.00000000	2.35561877
C	2.16769757	0.00000000	1.17403482
C	0.60425417	0.00000000	4.31789221
N	-0.58576202	0.00000000	-1.21165653
N	1.36665754	0.00000000	0.02366118
N	-0.73969677	0.00000000	1.09080088
N	-0.49236834	0.00000000	3.49496306
N	1.73663601	0.00000000	3.70112712
O	3.39454921	0.00000000	1.06404299
H	-0.05522824	0.00000000	-2.08234784
H	-1.45976252	0.00000000	3.77086439
H	-1.58928742	0.00000000	-1.23095229
H	1.88234753	0.00000000	-0.86972074
O	0.40804032	0.00000000	5.64051023
H	1.27822468	0.00000000	6.05041232
C	4.99398419	0.00000000	-3.69286823
C	2.20517073	0.00000000	-3.60524416
C	4.28422053	0.00000000	-4.83890470
C	4.24449795	0.00000000	-2.46114897
N	4.87470422	0.00000000	-1.28973472
N	2.91355198	0.00000000	-2.45162168
N	2.92788079	0.00000000	-4.80464612
O	0.98100198	0.00000000	-3.66009435
H	6.07429722	0.00000000	-3.70044435
H	2.37819396	0.00000000	-5.64932994
H	4.74504567	0.00000000	-5.81873275
H	4.33715281	0.00000000	-0.40613939
H	5.87850783	0.00000000	-1.25683978

HO-CC-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.19866600
O	-0.04885300	0.00000000	2.49977200
H	0.84181800	0.00000000	2.86295200
C	-0.01696900	0.00000000	-1.42041800
N	-1.21560100	0.00000000	-2.11774200
N	1.01902600	0.00000000	-2.21359600
C	-0.90374900	0.00000000	-3.44367100
H	-2.14239400	0.00000000	-1.72542800
C	0.48528500	0.00000000	-3.48283900
N	-1.78192800	0.00000000	-4.46265800
C	1.11607600	0.00000000	-4.76289800
C	-1.18847900	0.00000000	-5.63822700
N	0.17178100	0.00000000	-5.79603600
O	2.31624100	0.00000000	-5.02981700
N	-1.92426400	0.00000000	-6.76420800
H	0.56395200	0.00000000	-6.75006200
H	-1.51085400	0.00000000	-7.69628400
H	-2.92208000	0.00000000	-6.65445700
H	3.05948800	0.00000000	-6.61440400
N	3.47621600	0.00000000	-7.56014600
C	2.69747000	0.00000000	-8.63872000
H	4.47567800	0.00000000	-7.65879200
C	3.27984500	0.00000000	-9.95775400
N	1.37938800	0.00000000	-8.45476800
C	2.42651000	0.00000000	-11.00111500
H	4.35003000	0.00000000	-10.10548100
C	0.52649300	0.00000000	-9.50635800
N	1.08635000	0.00000000	-10.78980600
H	2.75462500	0.00000000	-12.03301700
O	-0.69425200	0.00000000	-9.40039600
H	0.43088300	0.00000000	-11.55540500

HO-CC$_2$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20687300
C	0.00000000	0.00000000	2.57488400
C	0.00000000	0.00000000	3.77700900
O	-0.07677700	0.00000000	5.07315500
H	0.80284600	0.00000000	5.46337300
C	-0.05964900	0.00000000	-1.41478700
N	-1.28024300	0.00000000	-2.07557200
N	0.95190800	0.00000000	-2.24241500
C	-1.00944400	0.00000000	-3.40844700
H	-2.19470600	0.00000000	-1.65470400
C	0.37997800	0.00000000	-3.49027400
N	-1.91644100	0.00000000	-4.40077300
C	0.97283600	0.00000000	-4.79055100
C	-1.35790400	0.00000000	-5.59401800
N	-0.00251300	0.00000000	-5.79351900
O	2.16337400	0.00000000	-5.09190600
N	-2.12669700	0.00000000	-6.69625200
H	0.36091200	0.00000000	-6.75934400
H	-1.74133100	0.00000000	-7.64073300
H	-3.12085900	0.00000000	-6.55626800
H	2.86489300	0.00000000	-6.70404600
N	3.25074700	0.00000000	-7.66174700
C	2.43615100	0.00000000	-8.71362600
H	4.24651100	0.00000000	-7.79250300
C	2.97407600	0.00000000	-10.05131200
N	1.12499300	0.00000000	-8.48523000
C	2.08619400	0.00000000	-11.06531800
H	4.03880100	0.00000000	-10.23412800
C	0.23756900	0.00000000	-9.50789700
N	0.75381400	0.00000000	-10.80902900
H	2.37884700	0.00000000	-12.10780400
O	-0.97908700	0.00000000	-9.36093800
H	0.07304800	0.00000000	-11.55227300

HO-CC$_3$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20863700
C	0.00000000	0.00000000	2.57056000
C	0.00466300	0.00000000	3.78158900
C	0.00991500	0.00000000	5.14548700
C	0.02106000	0.00000000	6.34863400
O	-0.04997300	0.00000000	7.64322300
H	0.83038400	0.00000000	8.03235200
C	-0.06680700	0.00000000	-1.41244400
N	-1.28954800	0.00000000	-2.06978700
N	0.94283900	0.00000000	-2.24386900
C	0.95863900	0.00000000	-4.79067800
N	-0.01965500	0.00000000	-5.79074900
C	-1.37452800	0.00000000	-5.58772700
N	-1.93110500	0.00000000	-4.39284900
C	-1.02231800	0.00000000	-3.40267600
C	0.36802200	0.00000000	-3.48803500
H	-2.20315800	0.00000000	-1.64678500
O	2.14797200	0.00000000	-5.09331600
N	-2.14583900	0.00000000	-6.68723600
H	0.34157700	0.00000000	-6.75777400
H	-1.76284700	0.00000000	-7.63304200
H	-3.13969800	0.00000000	-6.54456500
H	2.85084800	0.00000000	-6.71008000
N	3.23216600	0.00000000	-7.66893300
C	2.41286800	0.00000000	-8.71724400
H	4.22737500	0.00000000	-7.80391000
C	2.94506700	0.00000000	-10.05708100
N	1.10268200	0.00000000	-8.48321500
C	2.05289900	0.00000000	-11.06731800
H	4.00901000	0.00000000	-10.24432100

C	0.21106300	0.00000000	-9.50230400
N	0.72162300	0.00000000	-10.80533800
H	2.34104800	0.00000000	-12.11104200
O	-1.00502600	0.00000000	-9.34991400
H	0.03772500	0.00000000	-11.54573000

HO-CC$_4$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20920600
C	0.00000000	0.00000000	2.56888500
C	0.00000000	0.00000000	3.78182200
C	0.00000000	0.00000000	5.13922100
C	0.00000000	0.00000000	6.35149600
C	0.00000000	0.00000000	7.71357200
C	0.00000000	0.00000000	8.91717000
O	-0.08440500	0.00000000	10.20979100
H	0.79130300	0.00000000	10.60968300
C	-0.06452600	0.00000000	-1.41147300
N	-1.28519700	0.00000000	-2.07290700
N	0.94822200	0.00000000	-2.23999400
C	-1.01317400	0.00000000	-3.40453700
H	-2.20052900	0.00000000	-1.65347300
C	0.37802100	0.00000000	-3.48491300
N	-1.91735600	0.00000000	-4.39788400
C	0.97353600	0.00000000	-4.78604800
C	-1.35659600	0.00000000	-5.59108700
N	-0.00049700	0.00000000	-5.78936400
O	2.16384500	0.00000000	-5.08320700
N	-2.12368500	0.00000000	-6.69285700
H	0.36451500	0.00000000	-6.75525600
H	-1.73720100	0.00000000	-7.63748900
H	-3.11809700	0.00000000	-6.55370700
H	2.87433500	0.00000000	-6.69889300
N	3.25846700	0.00000000	-7.65623000
C	2.44176500	0.00000000	-8.70661700
H	4.25407100	0.00000000	-7.78824500
C	2.97708500	0.00000000	-10.04503200
N	1.13095900	0.00000000	-8.47562200
C	2.08725700	0.00000000	-11.05737800
H	4.04145000	0.00000000	-10.22982200
C	0.24181700	0.00000000	-9.49686800
N	0.75536900	0.00000000	-10.79855900
H	2.37791500	0.00000000	-12.10040000
O	-0.97467600	0.00000000	-9.34713800
H	0.07322500	0.00000000	-11.54059200

HO-CC$_5$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20944300
C	0.00000000	0.00000000	2.56809200
C	0.00000000	0.00000000	3.78161000
C	0.00000000	0.00000000	5.13671000
C	0.00000000	0.00000000	6.35089100
C	0.00000000	0.00000000	7.70681400
C	0.00000000	0.00000000	8.91950500
C	0.00000000	0.00000000	10.28084200
C	0.00000000	0.00000000	11.48462200
O	-0.08689100	0.00000000	12.77632700
H	0.78784400	0.00000000	13.17861600
C	-0.05268900	0.00000000	-1.41139100
N	-1.26703900	0.00000000	-2.08460500
N	0.96818100	0.00000000	-2.23029900
C	-0.98195500	0.00000000	-3.41330800
H	-2.18645500	0.00000000	-1.67409700
C	0.41028000	0.00000000	-3.47993000
N	-1.87567700	0.00000000	-4.41566400
C	1.01913000	0.00000000	-4.77546700
C	-1.30284700	0.00000000	-5.60337200
N	0.05534200	0.00000000	-5.78828600
O	2.21249600	0.00000000	-5.05925300
N	-2.05888000	0.00000000	-6.71231900
H	0.42965400	0.00000000	-6.75088800
H	-1.66328100	0.00000000	-7.65336700
H	-3.05464900	0.00000000	-6.58289800
H	2.93764400	0.00000000	-6.66704100
N	3.33080400	0.00000000	-7.62067900
C	2.52507600	0.00000000	-8.67943500
H	4.32776500	0.00000000	-7.74228900
C	3.07407200	0.00000000	-10.01217400
N	1.21187900	0.00000000	-8.46204300
C	2.19465000	0.00000000	-11.03359200
H	4.14023800	0.00000000	-10.18624800
C	0.33319500	0.00000000	-9.49237600
N	0.86011100	0.00000000	-10.78865400
H	2.49626600	0.00000000	-12.07350200
O	-0.88479100	0.00000000	-9.35476900
H	0.18569600	0.00000000	-11.53773700

HO-CC$_6$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20959000
C	0.00000000	0.00000000	2.56771900
C	0.00000000	0.00000000	3.78145100
C	0.00000000	0.00000000	5.13563800
C	0.00000000	0.00000000	6.35036300
C	0.00000000	0.00000000	7.70409500
C	0.00000000	0.00000000	8.91866200
C	0.00000000	0.00000000	10.27396700
C	0.00000000	0.00000000	11.48681700
C	0.00000000	0.00000000	12.84774000
C	0.00000000	0.00000000	14.05160500
O	-0.08576900	0.00000000	15.34279900
H	0.78887600	0.00000000	15.74542600
C	-0.06281700	0.00000000	-1.41061200
N	-1.28150100	0.00000000	-2.07580600
N	0.95289600	0.00000000	-2.23628400
C	-1.00495200	0.00000000	-3.40623400
H	-2.19851600	0.00000000	-1.65990500
C	0.38708700	0.00000000	-3.48181500
N	-1.90501500	0.00000000	-4.40256600
C	0.98767900	0.00000000	-4.78148900
C	-1.33977500	0.00000000	-5.59414300
N	0.01719800	0.00000000	-5.78789100
O	2.17878000	0.00000000	-5.07309400
N	-2.10296500	0.00000000	-6.69782900
H	0.38575600	0.00000000	-6.75274000
H	-1.71324600	0.00000000	-7.64141800
H	-3.09789600	0.00000000	-6.56195300

HO-CC$_7$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20966800
C	0.00000000	0.00000000	2.56749500
C	0.00000000	0.00000000	3.78132500
C	0.00000000	0.00000000	5.13507600
C	0.00000000	0.00000000	6.34998800
C	0.00000000	0.00000000	7.70287300
C	0.00000000	0.00000000	8.91796300
C	0.00000000	0.00000000	10.27113700
C	0.00000000	0.00000000	11.48584500
C	0.00000000	0.00000000	12.84082100
C	0.00000000	0.00000000	14.05374100
C	0.00000000	0.00000000	15.41440900
C	0.00000000	0.00000000	16.61832600
O	-0.08617600	0.00000000	17.90907300
H	0.78816100	0.00000000	18.31247900
C	-0.06397200	0.00000000	-1.41029300
N	-1.28284200	0.00000000	-2.07506100
N	0.95161900	0.00000000	-2.23637500
C	-1.00660300	0.00000000	-3.40549900
H	-2.19984700	0.00000000	-1.65911000
C	0.38561300	0.00000000	-3.48143200
N	-1.90674400	0.00000000	-4.40153000
C	0.98595800	0.00000000	-4.78145900

C	-1.34172200	0.00000000	-5.59335600
N	0.01522600	0.00000000	-5.78748100
O	2.17688000	0.00000000	-5.07316100
N	-2.10511700	0.00000000	-6.69665000
H	0.38371700	0.00000000	-6.75245200
H	-1.71571400	0.00000000	-7.64043500
H	-3.10001000	0.00000000	-6.56036600

HO-CC$_8$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20970800
C	0.00000000	0.00000000	2.56729100
C	0.00000000	0.00000000	3.78117700
C	0.00000000	0.00000000	5.13461900
C	0.00000000	0.00000000	6.34961600
C	0.00000000	0.00000000	7.70204200
C	0.00000000	0.00000000	8.91731300
C	0.00000000	0.00000000	10.26961400
C	0.00000000	0.00000000	11.48484800
C	0.00000000	0.00000000	12.83766800
C	0.00000000	0.00000000	14.05245100
C	0.00000000	0.00000000	15.40716000
C	0.00000000	0.00000000	16.62013200
C	0.00000000	0.00000000	17.98056900
C	0.00000000	0.00000000	19.18452300
O	-0.08505200	0.00000000	20.47502700
H	0.78936300	0.00000000	20.87840000
C	-0.05956000	0.00000000	-1.41031700
N	-1.27640500	0.00000000	-2.07901800
N	0.95877300	0.00000000	-2.23311500
C	-0.99571300	0.00000000	-3.40854500
H	-2.19486200	0.00000000	-1.66620100
C	0.39682900	0.00000000	-3.47979900
N	-1.89234600	0.00000000	-4.40762100
C	1.00160300	0.00000000	-4.77803600
C	-1.32323800	0.00000000	-5.59756400
N	0.03459800	0.00000000	-5.78720200
O	2.19382500	0.00000000	-5.06455700
N	-2.08279300	0.00000000	-6.70334100
H	0.40596200	0.00000000	-6.75130300
H	-1.69016700	0.00000000	-7.64591000
H	-3.07819900	0.00000000	-6.57063100

HO-CC$_9$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20973400
C	0.00000000	0.00000000	2.56722200
C	0.00000000	0.00000000	3.78111600
C	0.00000000	0.00000000	5.13447600
C	0.00000000	0.00000000	6.34946900
C	0.00000000	0.00000000	7.70178700
C	0.00000000	0.00000000	8.91707800
C	0.00000000	0.00000000	10.26913500
C	0.00000000	0.00000000	11.48448300
C	0.00000000	0.00000000	12.83664300
C	0.00000000	0.00000000	14.05188700
C	0.00000000	0.00000000	15.40464500
C	0.00000000	0.00000000	16.61942700
C	0.00000000	0.00000000	17.97408900
C	0.00000000	0.00000000	19.18706200
C	0.00000000	0.00000000	20.54742300
C	0.00000000	0.00000000	21.75139300
O	-0.08679000	0.00000000	23.04159300
H	0.78703300	0.00000000	23.44627300
C	-0.05908000	0.00000000	-1.41020400
N	-1.27499400	0.00000000	-2.08045000
N	0.96035100	0.00000000	-2.23179000
C	-0.99256500	0.00000000	-3.40954800
H	-2.19401600	0.00000000	-1.66891900
C	0.40013300	0.00000000	-3.47898600
N	-1.88780200	0.00000000	-4.40970000
C	1.00674800	0.00000000	-4.77644200
C	-1.31713900	0.00000000	-5.59902900
N	0.04082000	0.00000000	-5.78693200
O	2.19904500	0.00000000	-5.06171500
N	-2.07545000	0.00000000	-6.70552700
H	0.41366000	0.00000000	-6.75036800
H	-1.68175300	0.00000000	-7.64768100
H	-3.07098300	0.00000000	-6.57380700

HO-CC$_{10}$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.20976300
C	0.00000000	0.00000000	2.56709000
C	0.00611700	0.00000000	3.78100300
C	0.01293700	0.00000000	5.13418300
C	0.03044100	0.00000000	6.34908300
C	0.04992100	0.00000000	7.70108800
C	0.08110800	0.00000000	8.91600700
C	0.11579900	0.00000000	10.26740400
C	0.16177900	0.00000000	11.48192900
C	0.21292100	0.00000000	12.83276200
C	0.27407000	0.00000000	14.04660300
C	0.34209300	0.00000000	15.39688100
C	0.41818700	0.00000000	16.60975500
C	0.50288200	0.00000000	17.95970100
C	0.59303200	0.00000000	19.17114200
C	0.69354700	0.00000000	20.52186100
C	0.79588100	0.00000000	21.73050900
C	0.91066100	0.00000000	23.08617000
C	1.02129300	0.00000000	24.28503100
O	1.05195500	0.00000000	25.57761300
H	1.95875200	0.00000000	25.90180000
C	-0.05919700	0.00000000	-1.41007800
N	-1.27480500	0.00000000	-2.08087100
N	0.96068000	0.00000000	-2.23120300
C	1.00851200	0.00000000	-4.77571400
N	0.04293800	0.00000000	-5.78669000
C	-1.31519700	0.00000000	-5.59931700
N	-1.88617200	0.00000000	-4.41030500
C	-0.99169400	0.00000000	-3.40986900
C	0.40113600	0.00000000	-3.47854600
H	-2.19411100	0.00000000	-1.66993200
O	2.20087700	0.00000000	-5.06038200
N	-2.07303100	0.00000000	-6.70607300
H	0.41627100	0.00000000	-6.75000300
H	-1.67891200	0.00000000	-7.64812800
H	-3.06863100	0.00000000	-6.57475000

Table S7| Cartesian coordinates (in Å) of all H_2O^+-$(CC)_n$-GC systems, computed at ω-B97XD/6-311++G(d,p).

OH_2^+–GC

C	-0.44227900	1.75587100	0.00000000
C	1.65501600	2.45257300	0.00000000
C	2.21814200	1.17813400	0.00000000
C	1.33266100	0.04255600	0.00000000
C	3.80874800	2.49604700	0.00000000
N	-1.75328100	1.95209800	0.00000000
N	0.00000000	0.45606900	0.00000000
N	0.37999200	2.80705800	0.00000000
N	2.73348800	3.32468900	0.00000000
N	3.59700000	1.24410900	0.00000000
O	1.63682800	-1.13629600	0.00000000
O	5.14557900	3.05309500	0.00000000
H	-2.43109400	1.17620200	0.00000000
H	-2.07497700	2.90513500	0.00000000
H	-0.69830000	-0.31955500	0.00000000
H	2.69037700	4.33282800	0.00000000
H	5.64508900	2.80107400	0.79883700
H	5.64508900	2.80107400	-0.79883700
H	-2.24510800	-5.11735400	0.00000000
C	-2.51749600	-4.07215500	0.00000000
C	-3.15882300	-1.36362000	0.00000000
C	-3.80916100	-3.68401700	0.00000000
C	-1.52527300	-3.03355700	0.00000000
N	-0.22912000	-3.34375700	0.00000000
N	-1.85668200	-1.74238000	0.00000000
N	-4.12581600	-2.36504200	0.00000000
O	-3.52475700	-0.19126600	0.00000000
H	-5.08527100	-2.05325600	0.00000000
H	-4.63635100	-4.38214400	0.00000000
H	0.47566000	-2.60499300	0.00000000
H	0.06541700	-4.30418600	0.00000000

OH_2^+–CC–GC

C	-5.32050952	-0.36175666	0.00000000
C	-6.46441126	-0.70659223	0.00000000
O	-7.76366466	-1.09825942	0.00000000
H	-7.98860424	-2.04555189	0.00000000
H	-8.48043810	-0.44093554	0.00000000
C	-3.94795301	-0.02306271	0.00000000
N	-3.46741176	1.27444145	0.00000000
N	-2.99515189	-0.92214146	0.00000000
C	-2.10702599	1.17521869	0.00000000
H	-3.98654798	2.13781679	0.00000000
C	-1.84522231	-0.19832539	0.00000000
N	-1.24858020	2.19304753	0.00000000
C	-0.46733361	-0.62350966	0.00000000
C	0.01855983	1.79369045	0.00000000
N	0.39513578	0.47299061	0.00000000
O	-0.03754093	-1.76492891	0.00000000
N	0.99384902	2.69851929	0.00000000
H	1.40715750	0.23544823	0.00000000
H	1.98909517	2.44388776	0.00000000
H	0.71943167	3.66567563	0.00000000
H	1.73310008	-2.29766582	0.00000000
N	2.73296983	-2.51639910	0.00000000
C	3.63413892	-1.53472800	0.00000000
H	3.02741957	-3.47674680	0.00000000
C	5.03898436	-1.84039961	0.00000000
N	3.18703082	-0.27992503	0.00000000
C	5.89147931	-0.79527048	0.00000000
H	5.39896240	-2.85886240	0.00000000
C	4.05176266	0.76407076	0.00000000
N	5.41549387	0.47488929	0.00000000
H	6.96778738	-0.91087468	0.00000000
O	3.69980116	1.93988804	0.00000000
H	6.03570741	1.27024189	0.00000000

OH_2^+–$(CC)_2$–GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.21114000
C	0.00000000	0.00000000	2.56698400
C	0.00000000	0.00000000	3.76570800
O	0.00000000	0.00000000	5.11925600
H	0.83895900	0.00000000	5.61355600
H	-0.83773000	0.00000000	5.61497700
C	0.05312400	0.00000000	-1.40120300
N	-1.07268000	0.00000000	-2.21216700
N	1.17125200	0.00000000	-2.09468500
C	-0.62512800	0.00000000	-3.49553700
H	-2.03948800	0.00000000	-1.92925900
C	0.77214600	0.00000000	-3.38909700
N	-1.38134700	0.00000000	-4.59322300
C	1.54187700	0.00000000	-4.60858400
C	-0.66387900	0.00000000	-5.70958000
N	0.70910400	0.00000000	-5.72813300
O	2.75609600	0.00000000	-4.72803200
N	-1.28118300	0.00000000	-6.88965200
H	1.20171600	0.00000000	-6.64211200
H	-0.77553000	0.00000000	-7.78261200
H	-2.28630300	0.00000000	-6.87773500
H	3.72450000	0.00000000	-6.28995900
N	4.20161200	0.00000000	-7.19651800
C	3.49502600	0.00000000	-8.32604700
H	5.20562100	0.00000000	-7.22449800
C	4.16318100	0.00000000	-9.59957200
N	2.16683300	0.00000000	-8.22869500
C	3.38194300	0.00000000	-10.69887500
H	5.24067200	0.00000000	-9.67604100
C	1.38939600	0.00000000	-9.33894200
N	2.03092300	0.00000000	-10.57765200
H	3.77925700	0.00000000	-11.70588100
O	0.16266900	0.00000000	-9.31196900
H	1.42880200	0.00000000	-11.38663800

OH_2^+–$(CC)_3$–GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.21350799
C	0.00000001	-0.00000000	2.56186598
C	0.00000001	-0.00000000	3.77702798
C	0.00000001	-0.00000000	5.12935898
C	0.00000002	-0.00000000	6.32921797
O	0.00000002	-0.00000000	7.68122596
H	0.83839040	-0.00000000	8.17681606
H	-0.83783934	-0.00000000	8.17747586
C	0.00486299	0.00000000	-1.40080099
N	-1.15804215	0.00000000	-2.15919312
N	1.08815218	0.00000000	-2.14840086
C	-0.77389744	0.00000000	-3.46166107
H	-2.10900743	-0.00000000	-1.82697122
C	0.62712151	0.00000000	-3.42242890
N	-1.58192184	0.00000000	-4.52343515
C	1.33699698	0.00000000	-4.67644082
C	-0.91810134	0.00000000	-5.67130007
N	0.45197764	0.00000000	-5.75535991
O	2.54450908	0.00000000	-4.85590869
N	-1.59044884	0.00000000	-6.82245614
H	0.90010829	0.00000000	-6.69104185
H	-1.12757719	0.00000000	-7.73743008
H	-2.59374009	0.00000000	-6.76336425
H	3.43097987	0.00000000	-6.45163724
N	3.86936461	0.00000000	-7.37853627
C	3.11514517	0.00000000	-8.47652819
H	4.87123137	0.00000000	-7.44935335
C	3.72771106	0.00000000	-9.77819623
N	1.79250091	0.00000000	-8.32202109
C	2.89967251	0.00000000	-10.84244314

H	4.80092991	0.00000000	-9.90059331
C	0.96744236	0.00000000	-9.39723401
N	1.55506521	-0.00000000	-10.66287703
H	3.25229799	0.00000000	-11.86598615
O	-0.25677875	-0.00000000	-9.31717492
H	0.91855102	-0.00000000	-11.44501298

OH_2^+-(CC)$_4$-GC

C	-2.87343974	-0.33158817	0.00000000
C	-4.08013243	-0.20341296	0.00000000
C	-5.42047128	-0.06104181	0.00000000
C	-6.63109386	0.06755085	0.00000000
C	-7.96853800	0.20961452	0.00000000
C	-9.17785989	0.33806901	0.00000000
C	-10.52171497	0.48081366	0.00000000
C	-11.71525465	0.60759176	0.00000000
O	-13.05880444	0.75030398	0.00000000
H	-13.64117949	-0.03045302	0.00000000
H	-13.46382119	1.63621250	0.00000000
C	-1.47944300	-0.47871460	0.00000000
N	-0.85669423	-1.71973457	0.00000000
N	-0.61466804	0.51262645	0.00000000
C	0.48080637	-1.48570560	0.00000000
H	-1.29579283	-2.62628491	0.00000000
C	0.60044950	-0.09002757	0.00000000
N	1.44513408	-2.40970001	0.00000000
C	1.92570240	0.47265937	0.00000000
C	2.65970617	-1.88025925	0.00000000
N	2.89797342	-0.52873197	0.00000000
O	2.24270314	1.65237332	0.00000000
N	3.72910484	-2.67837381	0.00000000
H	3.87760869	-0.18921202	0.00000000
H	4.68945608	-2.32096189	0.00000000
H	3.55819640	-3.66862621	0.00000000
H	3.91932249	2.34980294	0.00000000
N	4.88948610	2.68416557	0.00000000
C	5.89818823	1.81438430	0.00000000
H	5.07033413	3.67211574	0.00000000
C	7.25946309	2.28087670	0.00000000
N	5.60020364	0.51661214	0.00000000
C	8.22655638	1.34124453	0.00000000
H	7.49877262	3.33423176	0.00000000
C	6.57816499	-0.42147433	0.00000000
N	7.90096595	0.02431607	0.00000000
H	9.28255171	1.57982202	0.00000000
O	6.36470962	-1.62947362	0.00000000
H	8.60860871	-0.69401804	0.00000000

OH_2^+-(CC)$_5$-GC

C	-1.94371649	0.40248842	0.00000000
C	-3.15240610	0.30101077	0.00000000
C	-4.49668170	0.18814976	0.00000000
C	-5.70977282	0.08630257	0.00000000
C	-7.04963495	-0.02618790	0.00000000
C	-8.26362092	-0.12811022	0.00000000
C	-9.60321299	-0.24057802	0.00000000
C	-10.81525979	-0.34233753	0.00000000
C	-12.16169678	-0.45538001	0.00000000
C	-13.35783555	-0.55580393	0.00000000
O	-14.70366667	-0.66879554	0.00000000
H	-15.12843406	-1.54553165	0.00000000
H	-15.26883235	0.12468350	0.00000000
C	-0.54587978	0.52538567	0.00000000
N	0.09389403	1.75772215	0.00000000
N	0.30467050	-0.47688622	0.00000000
C	1.42827733	1.50588626	0.00000000
H	-0.33413028	2.66949139	0.00000000
C	1.52931810	0.10982730	0.00000000
N	2.40546041	2.41795468	0.00000000
C	2.84595221	-0.46999414	0.00000000
C	3.61197308	1.87269334	0.00000000
N	3.83196148	0.51823464	0.00000000
O	3.14860849	-1.65416175	0.00000000
N	4.69346356	2.65620076	0.00000000
H	4.80652135	0.16619782	0.00000000
H	5.64838295	2.28585961	0.00000000
H	4.53614323	3.64859235	0.00000000
H	4.81138771	-2.36814266	0.00000000
N	5.77646522	-2.71876693	0.00000000
C	6.79924387	-1.86582713	0.00000000
H	5.94110169	-3.70952525	0.00000000
C	8.15300042	-2.35480983	0.00000000
N	6.52287974	-0.56343618	0.00000000
C	9.13534108	-1.43121433	0.00000000
H	8.37477414	-3.41200089	0.00000000
C	7.51575208	0.35864411	0.00000000
N	8.83144112	-0.10907382	0.00000000
H	10.18731098	-1.68701430	0.00000000
O	7.32238311	1.56986886	0.00000000
H	9.55068100	0.59758312	0.00000000

OH_2^+-(CC)$_6$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.21235900
C	0.00000000	0.00000000	2.56282300
C	0.00000000	0.00000000	3.77963100
C	0.00000000	0.00000000	5.12535600
C	0.00000000	0.00000000	6.34350400
C	0.00000000	0.00000000	7.68751900
C	0.00000000	0.00000000	8.90588100
C	0.00000000	0.00000000	10.25013200
C	0.00000000	0.00000000	11.46642600
C	0.00000000	0.00000000	12.81759800
C	0.00000000	0.00000000	14.01794300
O	0.00000000	0.00000000	15.36816800
H	0.83813100	0.00000000	15.86500300
H	-0.83805400	0.00000000	15.86509100
C	-0.03439500	0.00000000	-1.40434000
N	-1.22911000	0.00000000	-2.11216200
N	1.01309600	0.00000000	-2.19677000
C	-0.90344400	0.00000000	-3.43043400
H	-2.16292600	0.00000000	-1.73476200
C	0.49500900	0.00000000	-3.45392100
N	-1.76124800	0.00000000	-4.45689100
C	1.14635800	0.00000000	-4.73547400
C	-1.15031700	0.00000000	-5.63056500
N	0.21408600	0.00000000	-5.77491000
O	2.34573100	0.00000000	-4.97370000
N	-1.87243200	0.00000000	-6.75512400
H	0.61926800	0.00000000	-6.72810400
H	-1.44927800	0.00000000	-7.68727700
H	-2.87201200	0.00000000	-6.65384200
H	3.14711800	0.00000000	-6.58948800
N	3.55288900	0.00000000	-7.53332800
C	2.76091600	0.00000000	-8.60380500
H	4.55156700	0.00000000	-7.64007700
C	3.32791800	0.00000000	-9.92711700
N	1.44467900	0.00000000	-8.40346800
C	2.46280600	0.00000000	-10.96118100
H	4.39628500	0.00000000	-10.08668100
C	0.58160000	0.00000000	-9.44786600
N	1.12526300	0.00000000	-10.73450400
H	2.77879500	0.00000000	-11.99670000
O	-0.63873400	0.00000000	-9.32559000
H	0.46151100	0.00000000	-11.49348900

OH_2^+-(CC)$_7$-GC

C	0.02540012	0.38255736	0.00000000
C	-1.18497794	0.32366406	0.00000000
C	-2.53515562	0.25796855	0.00000000
C	-3.74991150	0.19886224	0.00000000
C	-5.09541170	0.13339432	0.00000000
C	-6.31154595	0.07422095	0.00000000
C	-7.65511744	0.00884687	0.00000000

C	-8.87187295	-0.05035673	0.00000000
C	-10.21430279	-0.11567526	0.00000000
C	-11.43112223	-0.17488197	0.00000000
C	-12.77389566	-0.24021722	0.00000000
C	-13.98863556	-0.29932274	0.00000000
C	-15.33828985	-0.36499279	0.00000000
C	-16.53714554	-0.42332544	0.00000000
O	-17.88553533	-0.48893396	0.00000000
H	-18.34118078	-1.35022014	0.00000000
H	-18.42269409	0.32399934	0.00000000
C	1.42718108	0.49141573	0.00000000
N	2.06782437	1.72336040	0.00000000
N	2.27561994	-0.51018831	0.00000000
C	3.40231317	1.47130122	0.00000000
H	1.63868785	2.63449248	0.00000000
C	3.50340811	0.07709605	0.00000000
N	4.37988454	2.38554727	0.00000000
C	4.81828685	-0.50188320	0.00000000
C	5.58503943	1.84091405	0.00000000
N	5.80466908	0.48675789	0.00000000
O	5.12384455	-1.68637696	0.00000000
N	6.66881242	2.62418878	0.00000000
H	6.77845498	0.13520526	0.00000000
H	7.62249260	2.25317003	0.00000000
H	6.51258182	3.61656789	0.00000000
H	6.77871488	-2.39411052	0.00000000
N	7.74323798	-2.74918360	0.00000000
C	8.76947561	-1.90082019	0.00000000
H	7.90377196	-3.74059900	0.00000000
C	10.12163136	-2.39568091	0.00000000
N	8.49857995	-0.59735906	0.00000000
C	11.10744123	-1.47606195	0.00000000
H	10.33850712	-3.45389115	0.00000000
C	9.49467415	0.32085705	0.00000000
N	10.80902741	-0.15266960	0.00000000
H	12.15850695	-1.73566806	0.00000000
O	9.30703599	1.53275108	0.00000000
H	11.53100687	0.55107592	0.00000000

OH_2^+-$(CC)_8$-GC

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.21137300
C	0.00000000	-0.00000000	2.56427799
C	0.00000001	-0.00000000	3.77996499
C	0.00000001	-0.00000000	5.12833800
C	0.00000001	-0.00000000	6.34534399
C	0.00000002	-0.00000000	7.69189899
C	0.00000001	-0.00000000	8.90954499
C	0.00000002	-0.00000000	10.25477699
C	0.00000002	-0.00000000	11.47287698
C	0.00000002	-0.00000000	12.81710198
C	0.00000003	-0.00000000	14.03523897
C	0.00000003	-0.00000000	15.37980697
C	0.00000003	-0.00000000	16.59588697
C	0.00000004	-0.00000000	17.94727996
C	0.00000004	-0.00000000	19.14750296
O	0.00000004	-0.00000000	20.49735496
H	0.83816736	-0.00000000	20.99437803
H	-0.83814326	-0.00000000	20.99439989
C	-0.04170497	0.00000000	-1.40646100
N	-1.24221598	0.00000000	-2.10395209
N	0.99811917	0.00000000	-2.20658392
C	-0.92825124	0.00000000	-3.42547306
H	-2.17217722	-0.00000000	-1.71736416
C	0.46847661	0.00000000	-3.46152297
N	-1.79665654	0.00000000	-4.44485313
C	1.10756108	0.00000000	-4.74749092
C	-1.19676103	0.00000000	-5.62289309
N	0.16598286	0.00000000	-5.77912599
O	2.30511909	0.00000000	-4.99902983
N	-1.92868444	0.00000000	-6.74282214
H	0.56270053	0.00000000	-6.73507396
H	-1.51311378	0.00000000	-7.67750710
H	-2.92727463	0.00000000	-6.63365922
H	3.08863714	0.00000000	-6.61252918
N	3.49043893	0.00000000	-7.55903119
C	2.69328958	0.00000000	-8.62544416
H	4.48847369	0.00000000	-7.67143924
C	3.25400556	0.00000000	-9.95188418
N	1.37810233	0.00000000	-8.41905610
C	2.38393109	0.00000000	-10.98165615
H	4.32162040	0.00000000	-10.11651623
C	0.50971486	0.00000000	-9.45885207
N	1.04744079	-0.00000000	-10.74859808
H	2.69488064	0.00000000	-12.01872216
O	-0.70987024	-0.00000000	-9.33111701
H	0.37998866	-0.00000000	-11.50422705

OH_2^+-$(CC)_9$-GC

C	2.10951272	0.41111117	0.00000000
C	0.89925685	0.36737167	0.00000000
C	-0.45364089	0.31847698	0.00000000
C	-1.66815198	0.27458369	0.00000000
C	-3.01664460	0.22584821	0.00000000
C	-4.23239988	0.18190996	0.00000000
C	-5.57925856	0.13323353	0.00000000
C	-6.79557647	0.08927494	0.00000000
C	-8.14125293	0.04064124	0.00000000
C	-9.35803254	-0.00333404	0.00000000
C	-10.70254975	-0.05192585	0.00000000
C	-11.91974309	-0.09591608	0.00000000
C	-13.26327595	-0.14447231	0.00000000
C	-14.48051426	-0.18846416	0.00000000
C	-15.82436690	-0.23703195	0.00000000
C	-17.03957654	-0.28095049	0.00000000
C	-18.39019477	-0.32976279	0.00000000
C	-19.58959472	-0.37310995	0.00000000
O	-20.93849208	-0.42186006	0.00000000
H	-21.40497549	-1.27749265	0.00000000
H	-21.46555215	0.39784115	0.00000000
C	3.51442065	0.50335756	0.00000000
N	4.16568718	1.72974158	0.00000000
N	4.35324899	-0.50472722	0.00000000
C	5.49840039	1.46663295	0.00000000
H	3.74301658	2.64387558	0.00000000
C	5.58785598	0.07282562	0.00000000
N	6.48420483	2.37381454	0.00000000
C	6.89688668	-0.51635983	0.00000000
C	7.68390692	1.81955121	0.00000000
N	7.89199017	0.46380717	0.00000000
O	7.19465580	-1.70363389	0.00000000
N	8.77579217	2.59367643	0.00000000
H	8.86232354	0.10419052	0.00000000
H	9.72560889	2.21457508	0.00000000
H	8.62791002	3.58726978	0.00000000
H	8.83357224	-2.42483854	0.00000000
N	9.79488646	-2.79084223	0.00000000
C	10.83098394	-1.95468848	0.00000000
H	9.94531560	-3.78388781	0.00000000
C	12.17736509	-2.46651498	0.00000000
N	10.57680322	-0.64799997	0.00000000
C	13.17457620	-1.55934224	0.00000000
H	12.38100300	-3.52745220	0.00000000
C	11.58400284	0.25803779	0.00000000
N	12.89274614	-0.23221197	0.00000000
H	14.22238999	-1.83218078	0.00000000
O	11.41185820	1.47209561	0.00000000
H	13.62333195	0.46257813	0.00000000

OH_2^+-$(CC)_{10}$-GC

C	21.08320933	-0.35019505	0.00000000
C	19.88368846	-0.31253237	0.00000000
C	18.53280517	-0.27011719	0.00000000
C	17.31750308	-0.23195901	0.00000000

C	15.97330650	-0.18975378	0.00000000
C	14.75600838	-0.15153293	0.00000000
C	13.41209466	-0.10933658	0.00000000
C	12.19486052	-0.07111774	0.00000000
C	10.84995529	-0.02889026	0.00000000
C	9.63313893	0.00931547	0.00000000
C	8.28711026	0.05157822	0.00000000
C	7.07070870	0.08977092	0.00000000
C	5.72366952	0.13206540	0.00000000
C	4.50764378	0.17024631	0.00000000
C	3.15962008	0.21257170	0.00000000
C	1.94406711	0.25073776	0.00000000
C	0.59457114	0.29310938	0.00000000
C	-0.61981241	0.33123872	0.00000000
C	-1.97359926	0.37374506	0.00000000
C	-3.18378588	0.41174263	0.00000000
O	22.43118905	-0.39251906	0.00000000
H	22.91315637	-1.23977509	0.00000000
H	22.96535686	0.42282824	0.00000000
C	-4.58951498	0.50004958	0.00000000
N	-5.24398532	1.72448767	0.00000000
N	-5.42536078	-0.51010005	0.00000000
C	-6.57605856	1.45790260	0.00000000
H	-4.82358559	2.63960238	0.00000000
C	-6.66206608	0.06441756	0.00000000
N	-7.56427223	2.36299342	0.00000000
C	-7.96902940	-0.52815883	0.00000000
C	-8.76225747	1.80586345	0.00000000
N	-8.96691761	0.44968638	0.00000000
O	-8.26393082	-1.71637129	0.00000000
N	-9.85640755	2.57743319	0.00000000
H	-9.93616662	0.08825628	0.00000000
H	-10.80505780	2.19601181	0.00000000
H	-9.71131690	3.57136658	0.00000000
H	-9.90404874	-2.43583862	0.00000000
N	-10.86427065	-2.80508499	0.00000000
C	-11.90300539	-1.97249532	0.00000000
H	-11.01006851	-3.79878769	0.00000000
C	-13.24791146	-2.48805458	0.00000000
N	-11.65233005	-0.66512194	0.00000000
C	-14.24753269	-1.58356985	0.00000000
H	-13.44856873	-3.54948209	0.00000000
C	-12.66184616	0.23808768	0.00000000
N	-13.96938997	-0.25571234	0.00000000
H	-15.29454014	-1.85922334	0.00000000
O	-12.49326394	1.45258545	0.00000000
H	-14.70182238	0.43703767	0.00000000