

## **Supporting Information**

# **Exploring $\pi$ - $\pi$ Interactions and Electron Transport in Complexes Involving Hexacationic Host and PAH Guest: A Promising Avenue for Molecular Devices**

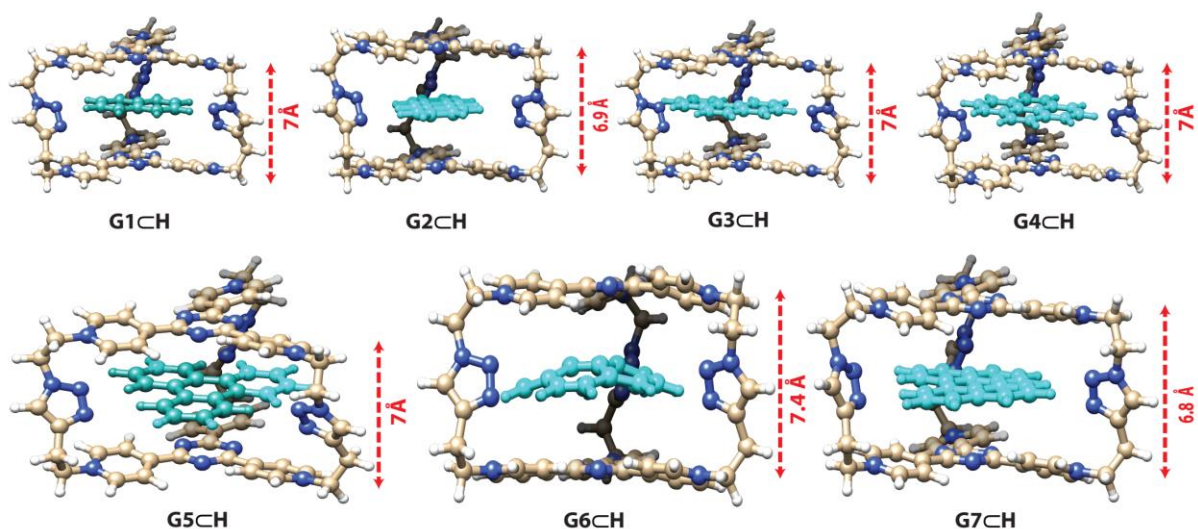
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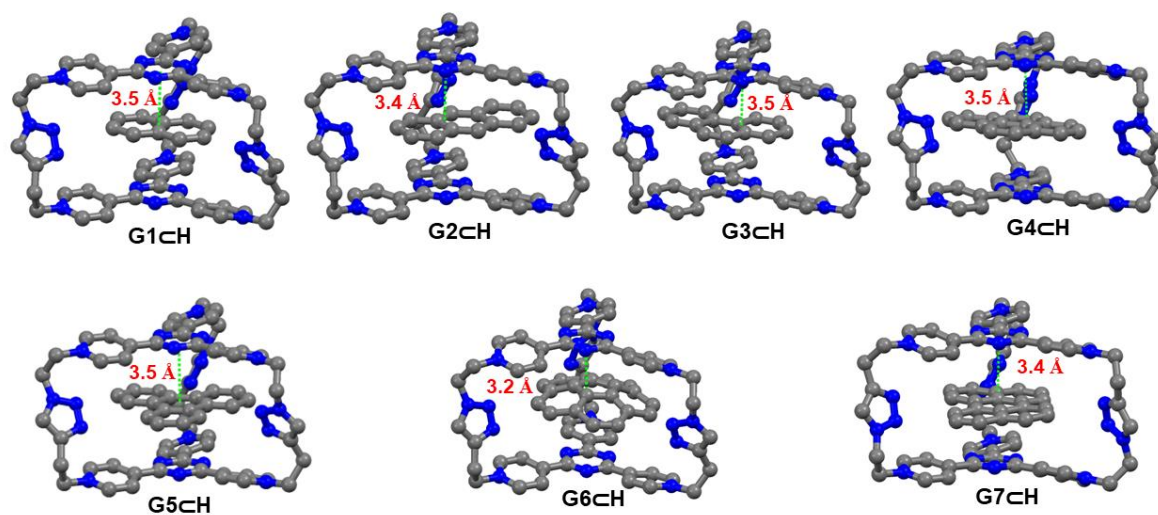
Guwahati-781039, India

## Table of Contents

S. No		Page No.
1	<b>Figure S1.</b> Centroids distances of Host ( <b>H</b> ) in complexes <b>G1cH</b> to <b>G7cH</b> calculated at the PBE0-D3BJ/def2-TZVP level of theory.	<b>S1</b>
2	<b>Figure S2.</b> Distances between host and guest in complexes <b>G1cH-G7cH</b> , calculated at the PBE0-D3BJ/def2-TZVP level of theory.	<b>S1</b>
3	<b>Table S1.</b> Interaction energy, $\Delta E$ (kcal mol <sup>-1</sup> ), of host-guest complexes <b>G1cH-G7cH</b> , calculated at the PBEh-3c/ def2-mSVP level of theory.	<b>S2</b>
4	<b>Figure S3.</b> Ab <i>initio</i> molecular dynamics simulation of complex ( <b>G1cH</b> ) calculated at the B97-3c/def2-mTZVP level of theory.	<b>S2</b>
5	<b>Figure S4.</b> Ab <i>initio</i> molecular dynamics simulation of complex ( <b>G2cH</b> ) calculated at the B97-3c/def2-mTZVP level of theory.	<b>S3</b>
6	<b>Figure S5.</b> Ab <i>initio</i> molecular dynamics simulation of complex ( <b>G3cH</b> ) calculated at the B97-3c/def2-mTZVP level of theory.	<b>S3</b>
7	<b>Figure S6.</b> Ab <i>initio</i> molecular dynamics simulation of complex ( <b>G4cH</b> ) calculated at the B97-3c/def2-mTZVP level of theory.	<b>S4</b>
8	<b>Figure S7.</b> Ab <i>initio</i> molecular dynamics simulation of complex ( <b>G5cH</b> ) calculated at the B97-3c/def2-mTZVP level of theory.	<b>S4</b>
9	<b>Figure S8.</b> Ab <i>initio</i> molecular dynamics simulation of complex ( <b>G6cH</b> ) calculated at the B97-3c/def2-mTZVP level of theory.	<b>S5</b>
10	<b>Figure S9:</b> I-V plot of host and host-guest complexes at the reverse and forward bias.	<b>S5</b>
11	<b>Table S2.</b> Conductance value and R <sup>2</sup> values of the host and host-guest complexes.	<b>S6</b>
12	<b>Figure S10:</b> Transmission spectra of the host ( <b>H</b> ) at voltage -1.0 eV to +1.0 eV.	<b>S6</b>
13	Optimized coordinates of the host ( <b>H</b> ) and host-guest complexes <b>G1cH-G7cH</b> calculated at the PBE0-D3BJ/def2-TZVP level of theory.	<b>S6-S30</b>



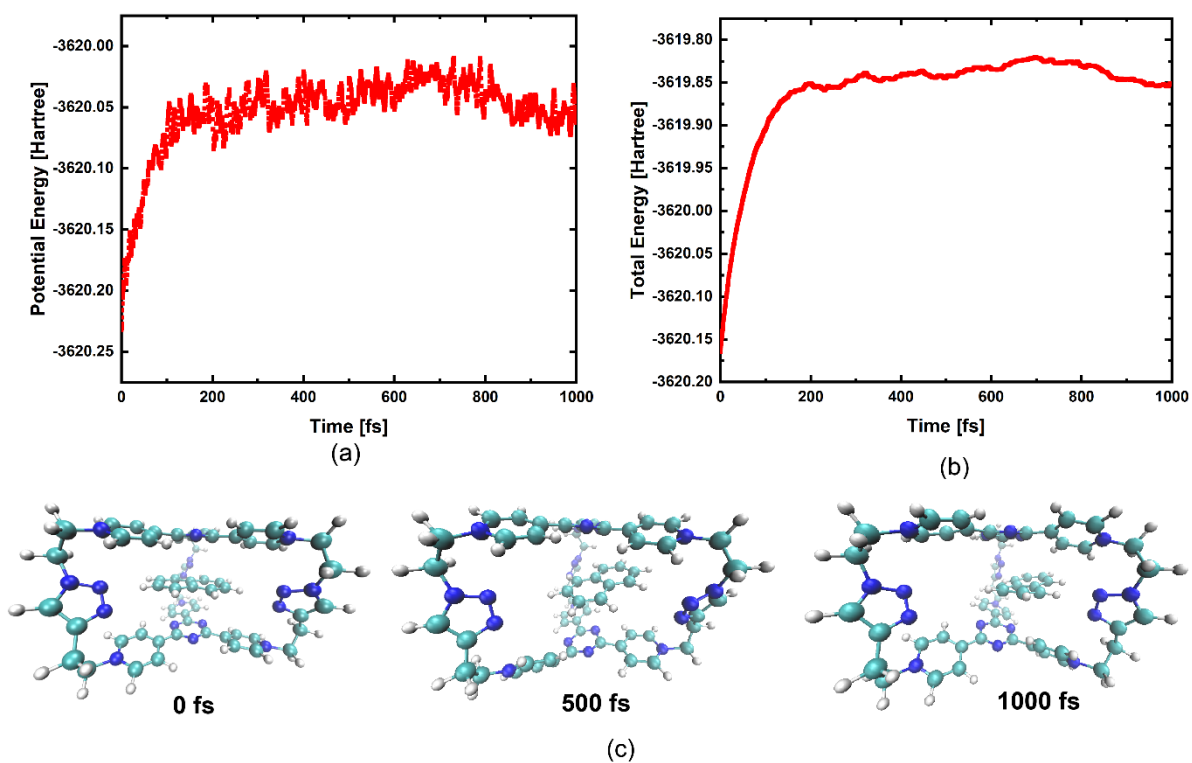
**Figure S1.** Centroids distances of Host (**H**) in complexes **G1cH** to **G7cH** calculated at the PBE0-D3BJ/def2-TZVP level of theory.



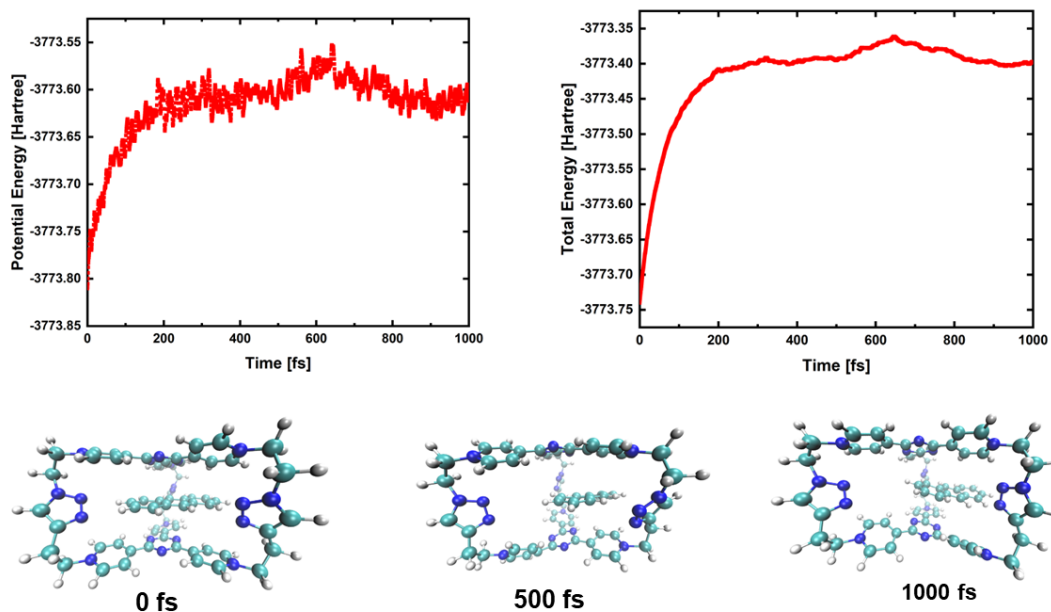
**Figure S2.** Distances between host and guest in complexes **G1cH**-**G7cH**, calculated at the PBE0-D3BJ/def2-TZVP level of theory.

**Table S1.** Interaction energy,  $\Delta E$  (kcal mol<sup>-1</sup>), of host-guest complexes **G1cH**-**G7cH**, calculated at the PBEh-3c/ def2-mSVP level of theory.

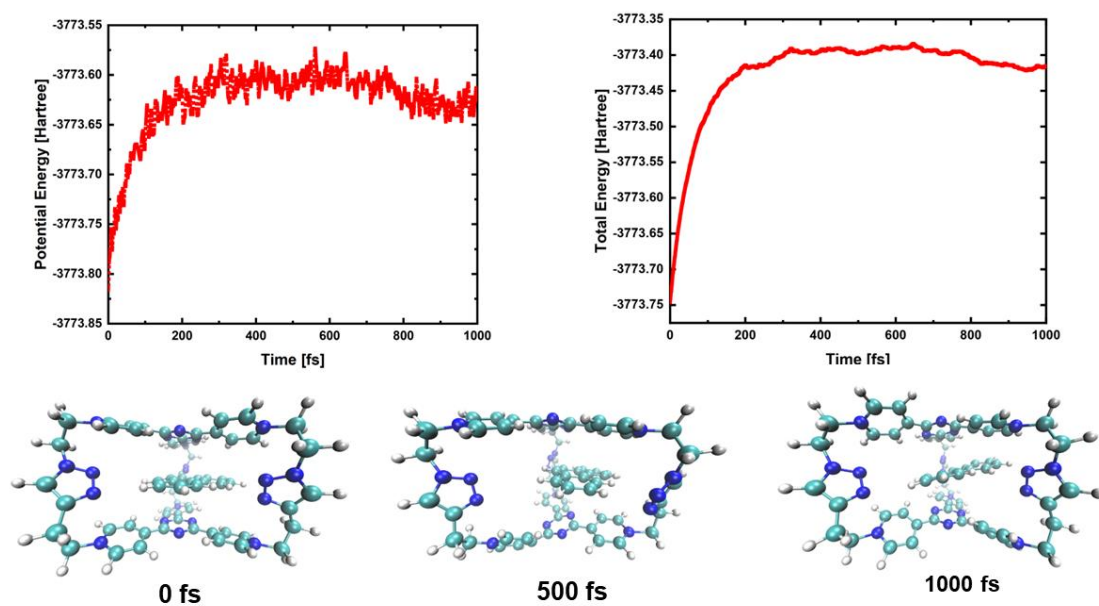
Complexes	$\Delta E$
<b>G1cH</b>	-34.02
<b>G2cH</b>	-44.02
<b>G3cH</b>	-50.42
<b>G4cH</b>	-43.14
<b>G5cH</b>	-43.38
<b>G6cH</b>	-41.00
<b>G7cH</b>	-51.96



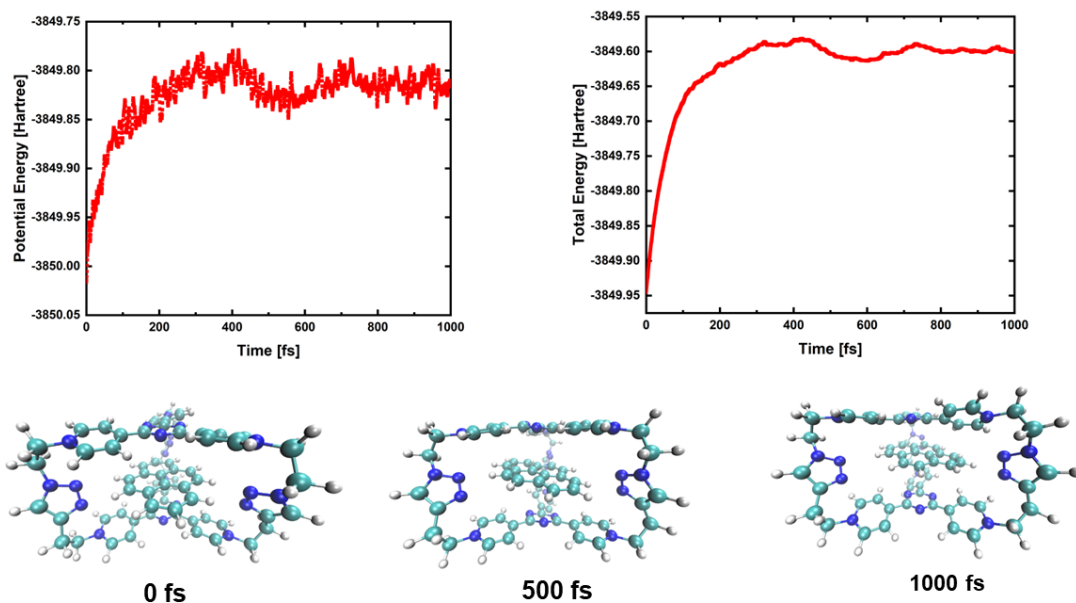
**Figure S3.** Ab *initio* molecular dynamics simulation of complex (**G1cH**) calculated at the B97-3c/def2-mTZVP level of theory.



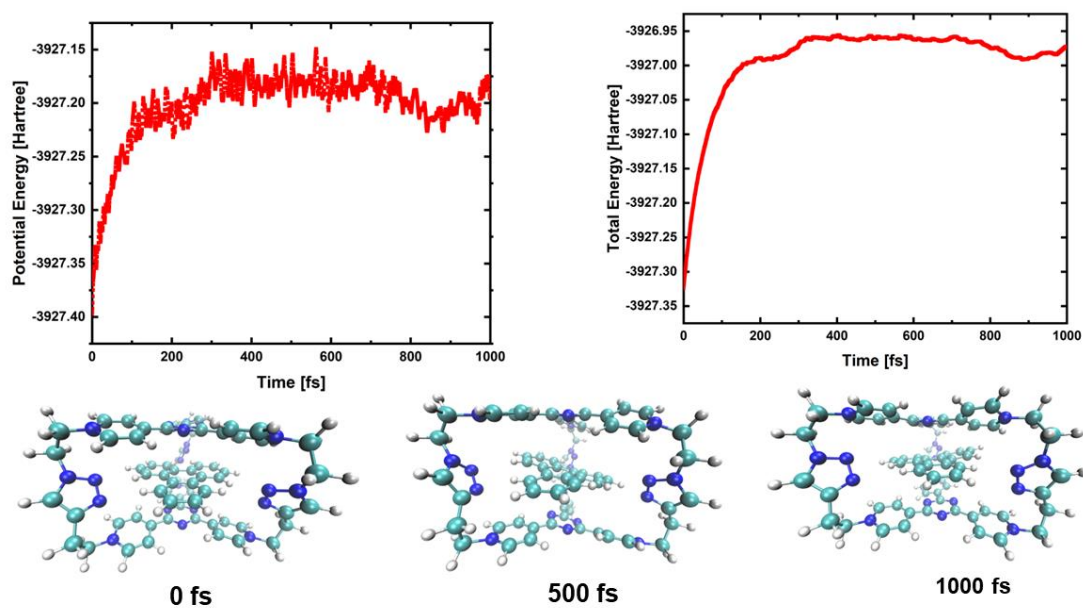
**Figure S4.** *Ab initio* molecular dynamics simulation of complex (**G2cH**) calculated at the B97-3c/def2-mTZVP level of theory.



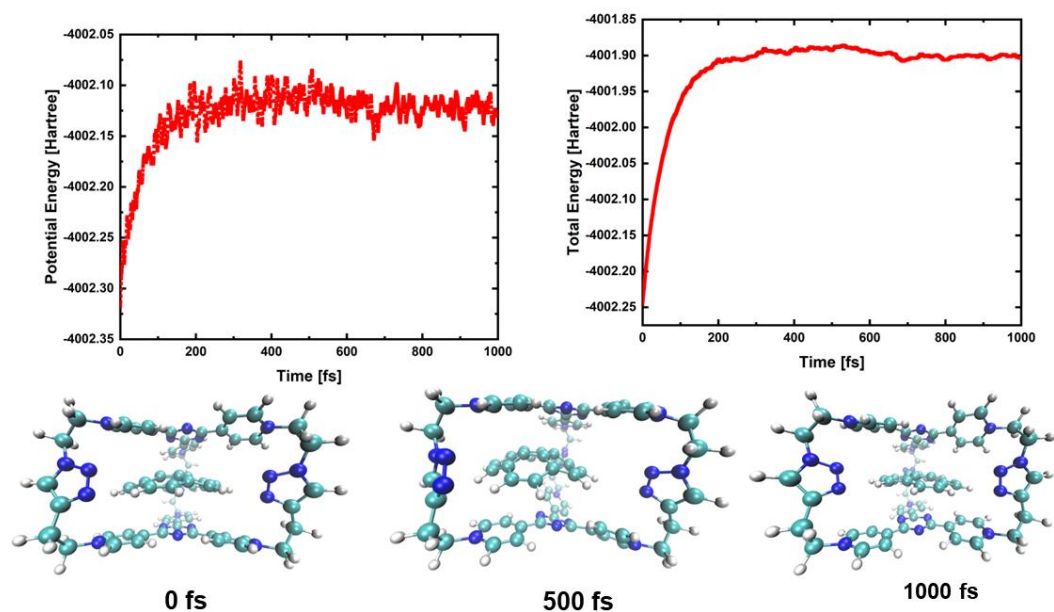
**Figure S5.** *Ab initio* molecular dynamics simulation of complex (**G3cH**) calculated at the B97-3c/def2-mTZVP level of theory.



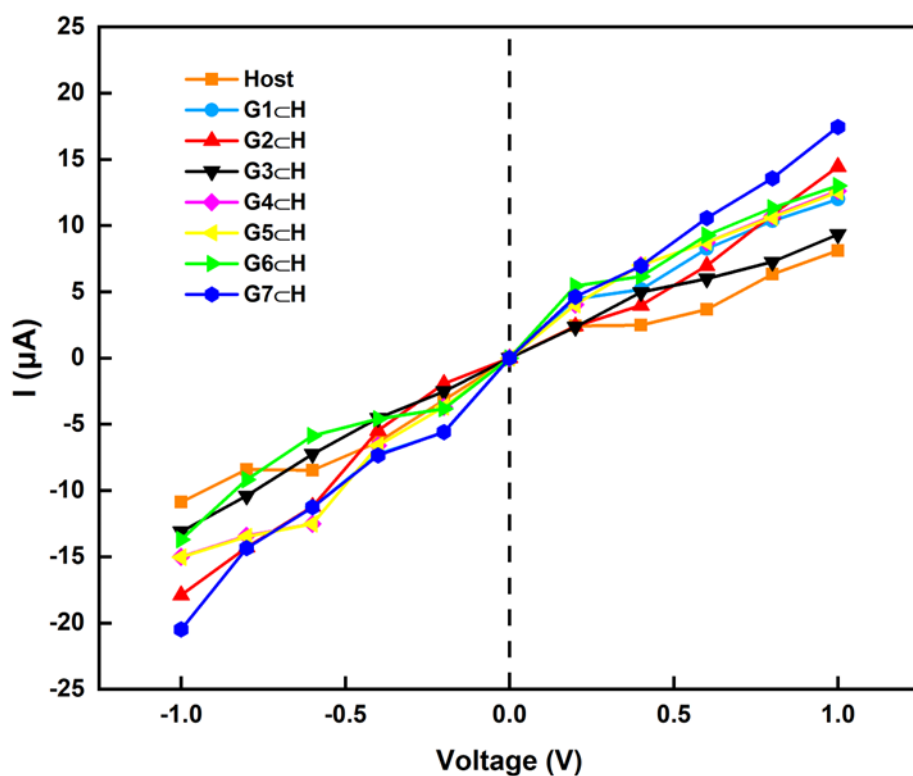
**Figure S6.** *Ab initio* molecular dynamics simulation of complex (G4cH) calculated at the B97-3c/def2-mTZVP level of theory.



**Figure S7.** *Ab initio* molecular dynamics simulation of complex (G5cH) calculated at the B97-3c/def2-mTZVP level of theory.



**Figure S8.** *Ab initio* molecular dynamics simulation of complex (G6cH) calculated at the B97-3c/def2-mTZVP level of theory.

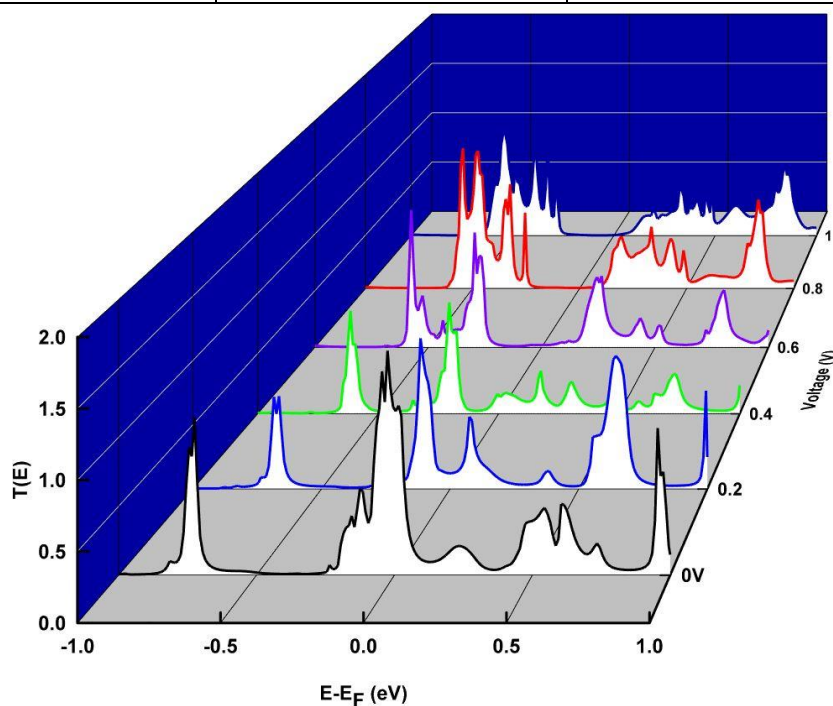


**Figure S9:** I-V plot of host and host-guest complexes at the reverse and forward bias.



**Table S2.** Conductance value and  $R^2$  values of the host and host-guest complexes.

Complexes	Conductance (S)* $10^{-5}$	$R^2$ -value
<b>H</b>	0.97	0.97
<b>G1cH</b>	1.61	0.97
<b>G2cH</b>	1.54	0.98
<b>G3cH</b>	1.11	0.98
<b>G4cH</b>	1.52	0.98
<b>G5cH</b>	1.51	0.98
<b>G6cH</b>	1.32	0.98
<b>G7cH</b>	1.84	0.99



**Figure S10:** Transmission spectra of the host (**H**) at voltage -1.0 eV to +1.0 eV.

**Optimized coordinates** of the host (**H**) and host-guest complexes **G1cH-G7cH** calculated at the PBE0-D3BJ/def2-TZVP level of theory.

**HOST (H) [+6]**

```

N      -4.77400000  2.32400000 -4.80700000
N      -0.38600000 -0.02100000 -5.16000000
N      1.88500000  0.59700000 -5.17400000
N      2.04600000 -4.38600000 -5.04900000
C      -4.43700000  1.09800000 -5.23900000
H      -5.25300000  0.43100000 -5.48700000
C      -3.11800000  0.73000000 -5.36200000

```



H	-2.87300000	-0.26300000	-5.71300000
C	-2.12000000	1.65000000	-5.05000000
C	-0.68400000	1.27500000	-5.12700000
C	0.91200000	-0.30900000	-5.18400000
C	1.30400000	-1.74200000	-5.17200000
C	0.38900000	-2.72000000	-4.80700000
H	-0.63300000	-2.46300000	-4.56400000
C	0.79200000	-4.03500000	-4.74000000
H	0.12500000	-4.83400000	-4.44600000
C	2.93900000	-3.46300000	-5.44100000
H	3.92400000	-3.82500000	-5.70700000
C	2.59900000	-2.13200000	-5.50300000
H	3.33600000	-1.40800000	-5.82400000
N	-4.55200000	2.57900000	2.52600000
N	-0.35400000	-0.13400000	2.66500000
N	1.95600000	0.31900000	2.64800000
N	1.70400000	-4.66200000	2.27900000
C	-4.27500000	1.31500000	2.18100000
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C	-2.99000000	0.82600000	2.26200000
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C	-0.55700000	1.18000000	2.69900000
C	0.91900000	-0.51500000	2.64100000
C	1.20200000	-1.97200000	2.55200000
C	0.22600000	-2.91200000	2.87400000
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C	2.66200000	-3.77500000	1.97800000
H	3.60200000	-4.17700000	1.62700000
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N	4.45000000	4.87600000	-4.86200000
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H	-4.17700000	4.19900000	-4.18700000
C	-2.49500000	2.92400000	-4.64300000
H	-1.75200000	3.67500000	-4.41400000
C	1.48600000	1.86500000	-5.14100000
C	2.53100000	2.91900000	-5.07900000
C	2.22200000	4.25000000	-5.34800000
H	1.22700000	4.54200000	-5.65600000
C	3.20500000	5.20600000	-5.24000000
H	3.02600000	6.25100000	-5.45700000
C	4.77300000	3.60100000	-4.61300000
H	5.79800000	3.40900000	-4.32700000
C	3.83600000	2.59900000	-4.72800000
H	4.12400000	1.57500000	-4.53300000
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N	4.85000000	4.37800000	2.45100000

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H	-1.51600000	3.65000000	3.40400000
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C	2.77000000	2.58800000	2.64000000
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H	1.54300000	4.25700000	2.04300000
C	3.60300000	4.77700000	2.16700000
H	3.48100000	5.80800000	1.86200000
C	5.09100000	3.11800000	2.85300000
H	6.11600000	2.87400000	3.10100000
C	4.07200000	2.19900000	2.94600000
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H	7.19500000	6.96800000	-1.03700000
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H	5.38500000	6.60000000	-5.55800000
H	6.44000000	5.47000000	-4.71100000
C	5.97900000	5.31900000	2.28800000
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H	5.56800000	6.32800000	2.27900000
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H	-6.28200000	3.74300000	-4.59300000
C	-5.93200000	3.09500000	2.38500000
H	-6.17000000	3.65200000	3.29200000
C	2.40200000	-6.85000000	-1.39700000
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N	2.11200000	-4.73000000	-1.93800000
N	1.77000000	-6.17100000	-0.41900000
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H	3.70400000	-7.07500000	-3.78000000
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H	1.58100000	-6.63300000	2.95400000
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H	-7.96300000	3.47900000	-0.92800000
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### **G1cH [+6]**

N	-5.57200000	1.19400000	-3.37500000
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H	-3.54400000	-1.38600000	-3.97600000
C	-2.88900000	0.59900000	-3.44200000
C	-1.44100000	0.27300000	-3.46400000
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C	-0.25600000	-3.69800000	-3.32500000
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H	-0.47300000	-5.84100000	-3.15800000
C	2.33500000	-4.32000000	-3.92500000
H	3.34000000	-4.63400000	-4.18100000
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H	2.68400000	-2.23000000	-4.12300000
N	-5.24800000	1.70300000	3.74800000
N	-1.08500000	-1.03800000	3.57800000
N	1.23100000	-0.62800000	3.53300000
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H	2.86900000	4.88400000	3.09300000
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H	3.57400000	0.14700000	4.09200000
C	5.69100000	5.35400000	0.09400000
H	6.46200000	6.10100000	0.20700000
C	4.75100000	5.13000000	-0.88500000
N	4.47400000	3.58400000	0.60900000
N	4.03000000	4.03800000	-0.51900000
N	5.47500000	4.37700000	0.99700000
C	4.47100000	5.90500000	-2.12700000
H	3.47400000	6.35300000	-2.06600000
H	5.17000000	6.74000000	-2.20300000
C	6.18600000	4.09400000	2.22500000

H	6.56900000	3.07300000	2.17500000
C	4.59500000	5.11700000	-3.43000000
H	4.43000000	5.77500000	-4.28400000
H	5.58200000	4.66900000	-3.53600000
C	5.35200000	4.30600000	3.48300000
H	5.98100000	4.14200000	4.36000000
H	4.96200000	5.32100000	3.53500000
H	7.04700000	4.76100000	2.28300000
C	-7.09300000	1.45200000	-0.71500000
N	-5.61500000	1.85900000	0.81700000
N	-5.79700000	1.29900000	-0.33600000
N	-6.78600000	2.36800000	1.20700000
C	-7.62900000	0.89700000	-1.99000000
H	-7.51400000	-0.19100000	-1.99600000
H	-8.70400000	1.08400000	-2.04900000
C	-7.01900000	1.48200000	-3.26300000
H	-7.50500000	1.05900000	-4.14200000
H	-7.13600000	2.56500000	-3.30300000
C	-6.62900000	2.22800000	3.69100000
H	-6.79800000	2.82900000	4.58600000
C	1.73200000	-7.81000000	-0.10000000
H	1.97200000	-8.86000000	-0.02900000
C	1.98800000	-6.86100000	-1.06100000
N	0.87700000	-5.86700000	0.51200000
N	1.44900000	-5.68900000	-0.63600000
N	1.04900000	-7.14600000	0.85400000
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H	3.11400000	-8.00900000	-2.44700000
C	1.92400000	-6.69700000	-3.60300000
H	2.53200000	-6.86700000	-4.49200000
H	1.04300000	-7.33500000	-3.67000000
C	1.14000000	-7.06200000	3.34100000
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H	-8.75900000	2.48100000	0.39300000
H	2.21600000	-7.23200000	3.34700000
C	0.49100000	-7.64800000	2.09200000
H	0.63700000	-8.72800000	2.11800000
H	-0.58500000	-7.46500000	2.08700000
H	-7.30700000	1.37600000	3.72500000
C	-6.88000000	3.09000000	2.45900000
H	-7.88800000	3.49700000	2.54100000
H	-6.19000000	3.93500000	2.42600000
C	-2.20100000	-1.84600000	-0.00500000
C	-0.89500000	-2.26200000	-0.00600000
C	0.16100000	-1.32200000	0.00800000
C	-0.15200000	0.06800000	0.04400000
C	-1.51000000	0.46100000	0.04800000
C	-2.51400000	-0.47100000	0.01600000
H	1.74700000	-2.77900000	-0.07300000

H	-3.00200000	-2.57600000	-0.02400000
H	-0.64800000	-3.32000000	-0.02000000
C	1.51800000	-1.71900000	-0.01900000
C	0.90600000	1.00500000	0.06800000
H	-1.75000000	1.52000000	0.06800000
H	-3.54900000	-0.14800000	-0.00200000
C	2.21200000	0.59200000	0.05500000
C	2.51900000	-0.78300000	0.00600000
H	0.66900000	2.06400000	0.09100000
H	3.01000000	1.32600000	0.07700000
H	3.55600000	-1.09900000	-0.01700000

### G2cH [+6]

N	-5.65400000	3.06000000	-4.33700000
N	-1.21100000	0.83000000	-3.91200000
N	1.04300000	1.50200000	-3.91000000
N	1.28100000	-3.47900000	-3.61100000
C	-5.26100000	1.77800000	-4.39200000
H	-6.03900000	1.04000000	-4.53400000
C	-3.93300000	1.44000000	-4.28200000
H	-3.64000000	0.40200000	-4.33400000
C	-2.98100000	2.44500000	-4.13100000
C	-1.53900000	2.11200000	-4.03200000
C	0.09100000	0.57500000	-3.86400000
C	0.51000000	-0.84600000	-3.77200000
C	-0.41300000	-1.83700000	-3.46400000
H	-1.44900000	-1.59400000	-3.27800000
C	0.00400000	-3.14600000	-3.37900000
H	-0.66800000	-3.95500000	-3.13300000
C	2.18500000	-2.54100000	-3.93400000
H	3.19100000	-2.88800000	-4.13500000
C	1.83000000	-1.21500000	-4.01500000
H	2.57300000	-0.47900000	-4.28700000
N	-5.73400000	4.04800000	2.66800000
N	-1.56700000	1.32200000	2.92900000
N	0.74500000	1.74100000	3.06200000
N	0.41900000	-3.23300000	3.40800000
C	-5.47300000	2.75600000	2.42200000
H	-6.32000000	2.13000000	2.17600000
C	-4.18900000	2.26800000	2.48800000
H	-4.00600000	1.22100000	2.28900000
C	-3.14500000	3.13300000	2.79000000
C	-1.74800000	2.63600000	2.86100000
C	-0.30400000	0.92400000	3.03400000
C	-0.05100000	-0.53400000	3.15600000
C	-1.10100000	-1.42200000	3.37800000
H	-2.11800000	-1.06800000	3.46600000
C	-0.83500000	-2.76400000	3.51000000
H	-1.61200000	-3.49200000	3.70700000

C	1.44600000	-2.39600000	3.19800000
H	2.42900000	-2.84200000	3.13600000
C	1.24100000	-1.04100000	3.08000000
H	2.08600000	-0.38400000	2.92900000
N	-0.66300000	3.11100000	-4.08900000
N	3.53700000	5.81800000	-4.13500000
C	-4.75600000	4.04400000	-4.19500000
H	-5.14500000	5.05300000	-4.16900000
C	-3.41200000	3.76600000	-4.10000000
H	-2.70400000	4.57800000	-4.00500000
C	0.61500000	2.75500000	-4.02100000
C	1.63900000	3.82900000	-4.07700000
C	1.29700000	5.12700000	-4.44400000
H	0.28400000	5.37800000	-4.72500000
C	2.26800000	6.10000000	-4.47100000
H	2.06200000	7.12100000	-4.76600000
C	3.89200000	4.57200000	-3.79500000
H	4.93400000	4.41700000	-3.55100000
C	2.96500000	3.55500000	-3.76800000
H	3.27500000	2.55600000	-3.49700000
N	-0.76700000	3.53400000	2.87500000
N	3.69000000	5.77700000	2.99500000
C	-4.74500000	4.89700000	2.99000000
H	-5.03100000	5.91900000	3.20600000
C	-3.44000000	4.46900000	3.05000000
H	-2.66100000	5.16900000	3.31800000
C	0.46100000	3.03600000	2.97500000
C	1.59300000	3.99800000	2.99900000
C	1.39800000	5.32500000	2.63700000
H	0.42000000	5.68200000	2.34700000
C	2.46700000	6.19100000	2.63400000
H	2.37300000	7.22900000	2.34500000
C	3.89600000	4.50800000	3.38400000
H	4.90100000	4.25200000	3.69600000
C	2.86800000	3.59600000	3.38800000
H	3.05800000	2.58100000	3.70800000
C	5.42100000	7.47800000	-0.54400000
H	6.20400000	8.21500000	-0.45500000
C	4.53700000	7.17800000	-1.55400000
N	4.12500000	5.79600000	0.06400000
N	3.76400000	6.14500000	-1.13000000
N	5.12100000	6.60100000	0.43500000
C	4.34900000	7.82700000	-2.88300000
H	3.36000000	8.29400000	-2.92800000
H	5.06800000	8.64000000	-2.99900000
C	5.75100000	6.41900000	1.72600000
H	6.14800000	5.40300000	1.77800000
C	4.53600000	6.91000000	-4.09100000
H	4.43200000	7.48200000	-5.01400000
H	5.52100000	6.44600000	-4.09300000
C	4.83400000	6.70900000	2.90900000



H	5.40900000	6.62200000	3.83300000
H	4.43200000	7.72000000	2.85900000
H	6.59900000	7.10100000	1.79200000
C	-7.36600000	3.56300000	-1.85600000
N	-5.96700000	4.04400000	-0.27100000
N	-6.09400000	3.42000000	-1.39900000
N	-7.15000000	4.58400000	0.02500000
C	-7.83600000	2.93100000	-3.12100000
H	-7.78200000	1.84200000	-3.02900000
H	-8.89100000	3.16300000	-3.28000000
C	-7.10000000	3.37700000	-4.38200000
H	-7.51600000	2.87500000	-5.25800000
H	-7.18800000	4.45100000	-4.53700000
C	-7.11100000	4.56200000	2.51400000
H	-7.32900000	5.20100000	3.37200000
C	1.44900000	-5.75300000	0.13800000
H	1.72700000	-6.78100000	0.31500000
C	1.70000000	-4.88800000	-0.90200000
N	0.49900000	-3.79900000	0.53500000
N	1.10200000	-3.70500000	-0.60700000
N	0.70900000	-5.03100000	1.00300000
C	2.49200000	-5.10100000	-2.14700000
H	3.38100000	-4.46400000	-2.13600000
H	2.86100000	-6.12900000	-2.17500000
C	1.72300000	-4.88200000	-3.44800000
H	2.35500000	-5.12400000	-4.30400000
H	0.83400000	-5.50900000	-3.50000000
C	0.66100000	-4.69000000	3.46900000
H	0.18200000	-5.07500000	4.37100000
C	-8.05500000	4.31900000	-0.93700000
H	-9.07500000	4.67000000	-0.89900000
H	1.73500000	-4.83900000	3.57000000
C	0.11100000	-5.43400000	2.25800000
H	0.30700000	-6.49700000	2.40700000
H	-0.97100000	-5.31300000	2.18000000
H	-7.78800000	3.70900000	2.55200000
C	-7.30300000	5.36700000	1.23400000
H	-8.31400000	5.77600000	1.24900000
H	-6.61100000	6.21000000	1.19400000
C	-3.52600000	-1.78600000	-0.34700000
C	-2.19200000	-1.51600000	-0.25700000
C	-1.71600000	-0.18200000	-0.36800000
C	-2.66300000	0.87700000	-0.56400000
C	-4.04400000	0.55400000	-0.66300000
C	-4.46100000	-0.74000000	-0.55800000
C	-0.35700000	0.12400000	-0.29700000
C	-2.20600000	2.19100000	-0.65500000
C	-0.84900000	2.49900000	-0.57700000
C	0.10100000	1.43600000	-0.40000000
C	1.48300000	1.76300000	-0.33100000
H	2.20000000	0.95900000	-0.19800000

C	1.90300000	3.05600000	-0.43400000
C	0.96600000	4.10400000	-0.61700000
C	-0.36800000	3.83300000	-0.68200000
H	0.35700000	-0.68600000	-0.17300000
H	-3.88600000	-2.80500000	-0.26400000
H	-1.47000000	-2.31100000	-0.09600000
H	-4.75100000	1.36000000	-0.83700000
H	-5.51400000	-0.98500000	-0.63600000
H	-2.93000000	2.98900000	-0.79500000
H	2.95700000	3.30400000	-0.37600000
H	1.33600000	5.11800000	-0.71800000
H	-1.08800000	4.63300000	-0.82400000

### **G3cH [+6]**

N	-5.33500000	1.53500000	-3.56800000
N	-0.90200000	-0.75300000	-3.59800000
N	1.35600000	-0.09300000	-3.62300000
N	1.55000000	-5.08900000	-3.73200000
C	-4.96000000	0.27100000	-3.82200000
H	-5.75400000	-0.43600000	-4.02800000
C	-3.63300000	-0.08500000	-3.82500000
H	-3.35400000	-1.10800000	-4.03500000
C	-2.66500000	0.88500000	-3.58100000
C	-1.22300000	0.53600000	-3.59000000
C	0.40000000	-1.01700000	-3.62200000
C	0.80800000	-2.44300000	-3.66300000
C	-0.11500000	-3.44700000	-3.39600000
H	-1.14000000	-3.20700000	-3.15100000
C	0.28800000	-4.76200000	-3.42700000
H	-0.38500000	-5.58100000	-3.21500000
C	2.45300000	-4.13800000	-4.02200000
H	3.44600000	-4.47800000	-4.28800000
C	2.11200000	-2.80600000	-3.98800000
H	2.85400000	-2.05900000	-4.23400000
N	-5.05500000	1.92200000	3.51600000
N	-0.90300000	-0.83200000	3.35200000
N	1.41500000	-0.43200000	3.39100000
N	1.05900000	-5.42000000	3.33200000
C	-4.81400000	0.66100000	3.12900000
H	-5.67400000	0.06600000	2.85400000
C	-3.53100000	0.16400000	3.09500000
H	-3.36200000	-0.85600000	2.78300000
C	-2.47100000	0.99100000	3.44400000
C	-1.07700000	0.48400000	3.40900000
C	0.36100000	-1.24200000	3.35400000
C	0.60700000	-2.70700000	3.34000000
C	-0.43600000	-3.60300000	3.55800000
H	-1.44100000	-3.25100000	3.74500000
C	-0.17900000	-4.95300000	3.55900000
H	-0.95000000	-5.69000000	3.74600000

C	2.08000000	-4.57600000	3.12400000
H	3.05100000	-5.02100000	2.95800000
C	1.88400000	-3.21400000	3.13300000
H	2.72500000	-2.55300000	2.97600000
N	-0.34500000	1.53200000	-3.60100000
N	3.83700000	4.24700000	-3.60400000
C	-4.42000000	2.48500000	-3.33400000
H	-4.79600000	3.48100000	-3.14600000
C	-3.07600000	2.19000000	-3.34400000
H	-2.35400000	2.97300000	-3.16400000
C	0.93200000	1.16700000	-3.61500000
C	1.95400000	2.24400000	-3.62600000
C	1.59000000	3.56400000	-3.87700000
H	0.56400000	3.82600000	-4.09400000
C	2.55400000	4.54400000	-3.86700000
H	2.33100000	5.58300000	-4.07200000
C	4.21200000	2.98200000	-3.37600000
H	5.26300000	2.81700000	-3.18600000
C	3.29200000	1.95700000	-3.39300000
H	3.62000000	0.94200000	-3.21900000
N	-0.09300000	1.37400000	3.45500000
N	4.37500000	3.59000000	3.50700000
C	-4.04800000	2.73100000	3.88400000
H	-4.31900000	3.72600000	4.21300000
C	-2.74500000	2.29500000	3.84800000
H	-1.95100000	2.96200000	4.15400000
C	1.13600000	0.86600000	3.43800000
C	2.27300000	1.82100000	3.48300000
C	2.06600000	3.17200000	3.23300000
H	1.07700000	3.54900000	3.01700000
C	3.13800000	4.03300000	3.23900000
H	3.03700000	5.08900000	3.03200000
C	4.59400000	2.29600000	3.79100000
H	5.61200000	2.01600000	4.03100000
C	3.56200000	1.38700000	3.77900000
H	3.76200000	0.35100000	4.01400000
C	5.88500000	5.56800000	0.00300000
H	6.69800000	6.27200000	0.09600000
C	4.92200000	5.38200000	-0.96100000
N	4.57300000	3.88000000	0.56300000
N	4.14200000	4.34100000	-0.56800000
N	5.62300000	4.62100000	0.92500000
C	4.67400000	6.14600000	-2.21600000
H	3.67800000	6.59800000	-2.18200000
H	5.37900000	6.97700000	-2.28500000
C	6.34100000	4.31500000	2.14500000
H	6.71500000	3.29100000	2.08100000
C	4.82600000	5.34300000	-3.50800000
H	4.68000000	5.99100000	-4.37300000
H	5.81500000	4.89400000	-3.58700000
C	5.52100000	4.51800000	3.41400000

H	6.16200000	4.35000000	4.28200000
H	5.13100000	5.53300000	3.47700000
H	7.20800000	4.97400000	2.20300000
C	-6.89000000	1.83200000	-0.94300000
N	-5.40600000	2.21700000	0.59000000
N	-5.59000000	1.68600000	-0.57700000
N	-6.57900000	2.69900000	1.00200000
C	-7.42800000	1.29900000	-2.22700000
H	-7.35600000	0.20700000	-2.23200000
H	-8.49400000	1.52600000	-2.30100000
C	-6.77700000	1.85900000	-3.48900000
H	-7.25500000	1.44200000	-4.37600000
H	-6.86600000	2.94400000	-3.53800000
C	-6.43400000	2.45200000	3.47400000
H	-6.60700000	3.01100000	4.39500000
C	1.87400000	-7.67300000	-0.17700000
H	2.16600000	-8.70900000	-0.09300000
C	2.06600000	-6.73100000	-1.16000000
N	0.93500000	-5.76500000	0.41600000
N	1.47700000	-5.58000000	-0.74600000
N	1.17700000	-7.02500000	0.77700000
C	2.79900000	-6.84000000	-2.45400000
H	3.69500000	-6.21100000	-2.42800000
H	3.15600000	-7.86300000	-2.58600000
C	1.97800000	-6.50600000	-3.69800000
H	2.57000000	-6.68700000	-4.59600000
H	1.07800000	-7.11600000	-3.76100000
C	1.28800000	-6.87900000	3.26000000
H	0.86300000	-7.33200000	4.15800000
C	-7.53700000	2.48900000	0.07700000
H	-8.55900000	2.80900000	0.20400000
H	2.36400000	-7.04300000	3.27900000
C	0.65300000	-7.52200000	2.03200000
H	0.84500000	-8.59500000	2.08500000
H	-0.43000000	-7.38700000	2.03200000
H	-7.11400000	1.60100000	3.46500000
C	-6.67600000	3.36900000	2.28100000
H	-7.68200000	3.77900000	2.37700000
H	-5.98000000	4.21100000	2.28600000
C	-3.11600000	-3.21400000	-0.15300000
C	-1.74300000	-3.25000000	-0.10700000
C	-0.99000000	-2.06200000	-0.10900000
C	-1.65100000	-0.80900000	-0.13500000
C	-3.05700000	-0.80100000	-0.19700000
C	-3.77100000	-1.97700000	-0.20800000
C	0.43700000	-2.11500000	-0.10500000
C	-0.86100000	0.40400000	-0.11100000
C	0.55500000	0.30600000	-0.11100000
C	1.17500000	-0.98000000	-0.11500000
C	1.33300000	1.47800000	-0.11600000
H	2.41500000	1.39400000	-0.12500000

C	0.74400000	2.72000000	-0.11400000
C	-0.65200000	2.82000000	-0.08900000
C	-1.43600000	1.68800000	-0.08600000
H	0.91400000	-3.09000000	-0.11900000
H	-3.69200000	-4.13200000	-0.15600000
H	-1.21200000	-4.19600000	-0.07100000
H	-3.60200000	0.13300000	-0.25500000
H	-4.85400000	-1.94700000	-0.26300000
H	2.26000000	-1.02800000	-0.12700000
H	1.36500000	3.60800000	-0.13600000
H	-1.12200000	3.79700000	-0.07400000
H	-2.51400000	1.79800000	-0.06400000

### **G4cH [+6]**

N	-4.76100000	2.46700000	-4.67800000
N	-0.39900000	0.00800000	-4.72800000
N	1.87700000	0.59900000	-4.78700000
N	1.97600000	-4.39300000	-4.86400000
C	-4.44000000	1.18200000	-4.89500000
H	-5.26300000	0.50000000	-5.06300000
C	-3.12600000	0.77300000	-4.91500000
H	-2.89500000	-0.26800000	-5.09600000
C	-2.11400000	1.70900000	-4.72400000
C	-0.68300000	1.30600000	-4.73700000
C	0.89600000	-0.29500000	-4.76300000
C	1.27400000	-1.73200000	-4.79200000
C	0.34800000	-2.72000000	-4.48100000
H	-0.66500000	-2.46500000	-4.20600000
C	0.73200000	-4.04200000	-4.51500000
H	0.05200000	-4.84900000	-4.27600000
C	2.88300000	-3.45700000	-5.18700000
H	3.86100000	-3.81200000	-5.48600000
C	2.56300000	-2.12000000	-5.15100000
H	3.30800000	-1.38700000	-5.42500000
N	-4.63200000	2.48600000	2.38800000
N	-0.39600000	-0.17900000	2.27200000
N	1.90700000	0.30100000	2.26000000
N	1.81900000	-4.68100000	2.19900000
C	-4.36400000	1.21100000	2.06800000
H	-5.21300000	0.58300000	1.83700000
C	-3.07100000	0.74000000	2.04800000
H	-2.88200000	-0.29300000	1.79000000
C	-2.02300000	1.60400000	2.34200000
C	-0.61300000	1.13300000	2.30300000
C	0.88200000	-0.54500000	2.25400000
C	1.19900000	-1.99800000	2.23900000
C	0.22000000	-2.95800000	2.47700000
H	-0.80100000	-2.67200000	2.69100000
C	0.56000000	-4.29200000	2.46100000
H	-0.15900000	-5.07500000	2.66400000

C	2.77900000	-3.77300000	1.97400000
H	3.77100000	-4.15500000	1.77700000
C	2.49900000	-2.42700000	1.99800000
H	3.29100000	-1.71400000	1.81900000
N	0.22800000	2.27600000	-4.76200000
N	4.52500000	4.83200000	-4.80200000
C	-3.80300000	3.38600000	-4.50000000
H	-4.13200000	4.40300000	-4.34100000
C	-2.47200000	3.03700000	-4.53000000
H	-1.71700000	3.79800000	-4.39400000
C	1.49400000	1.87200000	-4.78300000
C	2.55500000	2.91100000	-4.80800000
C	2.24700000	4.24700000	-5.05100000
H	1.23200000	4.55500000	-5.25700000
C	3.25400000	5.18400000	-5.04900000
H	3.07300000	6.23200000	-5.25100000
C	4.84600000	3.55100000	-4.58100000
H	5.89100000	3.33900000	-4.40200000
C	3.88300000	2.56800000	-4.59000000
H	4.16700000	1.54000000	-4.41800000
N	0.34300000	2.05700000	2.30700000
N	4.76500000	4.39500000	2.30700000
C	-3.63800000	3.33100000	2.70500000
H	-3.92400000	4.33700000	2.98500000
C	-2.32600000	2.92000000	2.68100000
H	-1.54500000	3.62000000	2.94400000
C	1.58700000	1.59000000	2.28700000
C	2.70000000	2.57600000	2.30400000
C	2.46600000	3.91700000	2.02800000
H	1.47000000	4.27000000	1.80200000
C	3.51900000	4.80200000	2.02500000
H	3.39300000	5.85300000	1.80100000
C	5.01100000	3.11000000	2.60900000
H	6.03300000	2.85500000	2.86100000
C	4.00000000	2.17800000	2.60600000
H	4.22300000	1.15000000	2.85700000
C	6.52400000	6.29600000	-1.16000000
H	7.31500000	7.02000000	-1.03600000
C	5.64500000	6.04600000	-2.18800000
N	5.20200000	4.60800000	-0.62700000
N	4.85700000	5.00800000	-1.80900000
N	6.20400000	5.38600000	-0.21800000
C	5.46200000	6.75400000	-3.48800000
H	4.49900000	7.27600000	-3.48900000
H	6.22000000	7.53200000	-3.59200000
C	6.82000000	5.14400000	1.07000000
H	7.23500000	4.13400000	1.07300000
C	5.57200000	5.87900000	-4.73500000
H	5.47100000	6.49400000	-5.63100000
H	6.53400000	5.37200000	-4.78300000
C	5.88600000	5.35900000	2.25400000

H	6.45800000	5.25400000	3.17800000
H	5.45600000	6.36000000	2.24000000
H	7.65600000	5.83600000	1.18300000
C	-6.46100000	2.75800000	-2.09100000
N	-5.01600000	3.05400000	-0.50400000
N	-5.16200000	2.64000000	-1.72200000
N	-6.21300000	3.43200000	-0.06300000
C	-6.94600000	2.30800000	-3.42800000
H	-6.94700000	1.21400000	-3.47000000
H	-7.98900000	2.60400000	-3.56100000
C	-6.18900000	2.87000000	-4.62800000
H	-6.65200000	2.52100000	-5.55300000
H	-6.21000000	3.95800000	-4.63400000
C	-6.03200000	2.96900000	2.38000000
H	-6.22500000	3.44100000	3.34600000
C	2.56700000	-7.03800000	-1.39500000
H	2.77200000	-8.09600000	-1.35700000
C	2.74100000	-6.09100000	-2.38000000
N	1.88000000	-5.06900000	-0.67700000
N	2.31000000	-4.90300000	-1.88700000
N	2.03800000	-6.35200000	-0.36200000
C	3.31400000	-6.21300000	-3.75000000
H	4.23500000	-5.62600000	-3.81700000
H	3.60600000	-7.24800000	-3.93800000
C	2.36900000	-5.82300000	-4.88500000
H	2.84900000	-6.00800000	-5.84800000
H	1.44900000	-6.40600000	-4.85400000
C	2.14800000	-6.12200000	2.12200000
H	1.77100000	-6.59900000	3.03000000
C	-7.15200000	3.27500000	-1.01900000
H	-8.19000000	3.53300000	-0.87400000
H	3.23400000	-6.20600000	2.12900000
C	1.55000000	-6.83400000	0.91600000
H	1.80800000	-7.89000000	1.00300000
H	0.45900000	-6.76800000	0.92100000
H	-6.67600000	2.09400000	2.30200000
C	-6.33500000	3.97400000	1.27400000
H	-7.36300000	4.31200000	1.41600000
H	-5.69300000	4.85400000	1.35100000
C	-1.75200000	-2.55900000	-1.13400000
C	-0.36600000	-2.61400000	-1.15000000
C	0.39500000	-1.44400000	-1.20100000
C	-0.26700000	-0.19200000	-1.21600000
C	-1.68500000	-0.14400000	-1.20600000
C	-2.40700000	-1.33900000	-1.17200000
C	1.82500000	-1.46600000	-1.25100000
C	0.48200000	1.01200000	-1.24700000
C	1.90200000	0.96300000	-1.27400000
C	2.54200000	-0.31600000	-1.28300000
C	2.61700000	2.16100000	-1.31200000
H	3.70200000	2.14200000	-1.33100000



C	1.95700000	3.38100000	-1.33200000
C	0.57400000	3.43600000	-1.30100000
C	-0.18500000	2.26400000	-1.25700000
C	-1.61300000	2.27900000	-1.24200000
C	-2.32700000	1.12800000	-1.22900000
H	-3.40900000	1.17300000	-1.25000000
H	-2.13000000	3.23200000	-1.25000000
H	2.31900000	-2.43100000	-1.28400000
H	-2.32900000	-3.47600000	-1.10000000
H	0.14700000	-3.56700000	-1.12000000
H	-3.49100000	-1.30300000	-1.17500000
H	3.62600000	-0.34800000	-1.32600000
H	2.54500000	4.29000000	-1.38700000
H	0.06500000	4.39500000	-1.31900000

### G5cH [+6]

N	-5.53100000	1.05400000	-3.48400000
N	-0.98400000	-0.99600000	-3.68300000
N	1.23300000	-0.21200000	-3.72300000
N	1.72800000	-5.17700000	-3.86500000
C	-5.09900000	-0.17300000	-3.81900000
H	-5.86000000	-0.90700000	-4.05100000
C	-3.75600000	-0.45800000	-3.86900000
H	-3.43000000	-1.45100000	-4.14500000
C	-2.83300000	0.54500000	-3.58600000
C	-1.37500000	0.27300000	-3.63500000
C	0.33000000	-1.18600000	-3.72700000
C	0.82200000	-2.58500000	-3.78000000
C	-0.03600000	-3.64400000	-3.51800000
H	-1.07400000	-3.46900000	-3.27300000
C	0.44800000	-4.93200000	-3.55800000
H	-0.17200000	-5.79400000	-3.35400000
C	2.57000000	-4.17000000	-4.14600000
H	3.58300000	-4.44600000	-4.41200000
C	2.14700000	-2.86300000	-4.10300000
H	2.84100000	-2.06800000	-4.33600000
N	-5.21100000	1.45400000	3.62600000
N	-0.92600000	-1.08700000	3.41100000
N	1.36800000	-0.56600000	3.36200000
N	1.30800000	-5.55100000	3.23800000
C	-4.91300000	0.19800000	3.26200000
H	-5.74700000	-0.44600000	3.02100000
C	-3.60800000	-0.23300000	3.21000000
H	-3.39000000	-1.25000000	2.91700000
C	-2.58400000	0.65500000	3.51900000
C	-1.16700000	0.21800000	3.45800000
C	0.35700000	-1.42900000	3.36500000
C	0.68700000	-2.87600000	3.32000000
C	-0.26700000	-3.83600000	3.64500000

H	-1.26500000	-3.55000000	3.94500000
C	0.07400000	-5.16700000	3.60500000
H	-0.62100000	-5.95300000	3.87000000
C	2.24300000	-4.64300000	2.92500000
H	3.21500000	-5.02500000	2.64700000
C	1.96400000	-3.29600000	2.96800000
H	2.73300000	-2.58100000	2.71600000
N	-0.55300000	1.31600000	-3.62700000
N	3.49900000	4.23000000	-3.64100000
C	-4.66100000	2.03500000	-3.21300000
H	-5.08300000	2.99800000	-2.96000000
C	-3.30400000	1.81200000	-3.26600000
H	-2.61900000	2.61900000	-3.04900000
C	0.74200000	1.02100000	-3.67300000
C	1.70700000	2.14800000	-3.66700000
C	1.28200000	3.45300000	-3.89700000
H	0.24300000	3.67100000	-4.10000000
C	2.20200000	4.47400000	-3.88600000
H	1.93200000	5.50400000	-4.08100000
C	3.93100000	2.98200000	-3.42300000
H	4.99000000	2.86200000	-3.24200000
C	3.05800000	1.91800000	-3.44100000
H	3.42800000	0.91700000	-3.26800000
N	-0.22900000	1.15900000	3.46000000
N	4.11900000	3.60100000	3.43200000
C	-4.24000000	2.32200000	3.95300000
H	-4.55500000	3.31000000	4.26400000
C	-2.91700000	1.95200000	3.89900000
H	-2.15200000	2.66700000	4.16900000
C	1.02300000	0.71500000	3.41100000
C	2.11100000	1.72500000	3.41900000
C	1.83400000	3.06100000	3.15900000
H	0.82600000	3.38600000	2.94200000
C	2.86100000	3.97700000	3.16200000
H	2.70400000	5.02600000	2.95400000
C	4.40700000	2.31800000	3.70900000
H	5.43900000	2.09200000	3.94500000
C	3.42400000	1.35700000	3.70000000
H	3.67800000	0.33200000	3.92800000
C	5.52300000	5.67400000	-0.03400000
H	6.26800000	6.44800000	0.07200000
C	4.59100000	5.40900000	-1.01000000
N	4.37200000	3.86600000	0.49600000
N	3.90900000	4.29600000	-0.63400000
N	5.34300000	4.69700000	0.87600000
C	4.28200000	6.16000000	-2.26000000
H	3.26700000	6.56700000	-2.20500000
H	4.94500000	7.02400000	-2.34100000
C	6.06500000	4.44600000	2.10700000
H	6.51100000	3.45100000	2.05000000
C	4.44300000	5.36700000	-3.55400000

H	4.25700000	6.01100000	-4.41500000
H	5.44900000	4.95900000	-3.65200000
C	5.21200000	4.59300000	3.36100000
H	5.84500000	4.45900000	4.24000000
H	4.76200000	5.58300000	3.42000000
H	6.88200000	5.16500000	2.17600000
C	-7.06500000	1.24500000	-0.81300000
N	-5.60100000	1.73400000	0.70900000
N	-5.75500000	1.19100000	-0.45700000
N	-6.80200000	2.13200000	1.13100000
C	-7.57500000	0.68000000	-2.09400000
H	-7.41900000	-0.40300000	-2.11000000
H	-8.65600000	0.82600000	-2.15300000
C	-6.98600000	1.29800000	-3.36000000
H	-7.46300000	0.87100000	-4.24300000
H	-7.13500000	2.37700000	-3.38700000
C	-6.61700000	1.90900000	3.60400000
H	-6.80500000	2.46600000	4.52300000
C	2.18600000	-7.73000000	-0.33500000
H	2.48900000	-8.76400000	-0.27000000
C	2.36400000	-6.77000000	-1.30300000
N	1.23500000	-5.84100000	0.29600000
N	1.76700000	-5.63100000	-0.86500000
N	1.48900000	-7.10600000	0.63400000
C	3.09000000	-6.84900000	-2.60300000
H	3.95200000	-6.17600000	-2.58600000
H	3.49900000	-7.85400000	-2.73200000
C	2.24300000	-6.56400000	-3.84100000
H	2.83900000	-6.70500000	-4.74400000
H	1.38300000	-7.22900000	-3.90000000
C	1.61700000	-6.99100000	3.11800000
H	1.23900000	-7.49200000	4.01100000
C	-7.74900000	1.85500000	0.21300000
H	-8.79100000	2.10200000	0.34800000
H	2.70100000	-7.09600000	3.10900000
C	0.98700000	-7.63100000	1.88600000
H	1.20500000	-8.69900000	1.92100000
H	-0.09900000	-7.52000000	1.89900000
H	-7.25000000	1.02200000	3.61400000
C	-6.93100000	2.80100000	2.40800000
H	-7.96100000	3.14400000	2.51200000
H	-6.29200000	3.68600000	2.40200000
C	1.01400000	-1.06500000	-0.21000000
C	2.03500000	-2.02500000	-0.30900000
C	3.36300000	-1.66300000	-0.32500000
C	3.71500000	-0.31700000	-0.23500000
C	2.73200000	0.64400000	-0.16200000
C	1.36900000	0.30100000	-0.16500000
C	-0.39000000	-1.45400000	-0.16700000
C	-0.77300000	-2.80600000	-0.16600000
C	-2.09900000	-3.17700000	-0.15600000

C	-3.09200000	-2.19900000	-0.15900000
C	-2.74200000	-0.86800000	-0.14000000
C	-1.39600000	-0.46400000	-0.12500000
H	1.79200000	-3.07700000	-0.39100000
H	4.13100000	-2.42300000	-0.40800000
H	4.75900000	-0.02500000	-0.23100000
H	3.03400000	1.68100000	-0.09700000
H	-0.02300000	-3.58600000	-0.16800000
H	-2.36700000	-4.22800000	-0.15500000
H	-4.13800000	-2.48500000	-0.17700000
H	-3.53500000	-0.13100000	-0.15400000
C	-2.00600000	1.95200000	0.00700000
C	-1.02900000	0.94600000	-0.07900000
C	0.33100000	1.32300000	-0.12100000
C	0.65200000	2.69100000	-0.13200000
C	-0.32500000	3.65900000	-0.06700000
C	-1.66600000	3.28600000	0.02000000
H	-3.05400000	1.69100000	0.07000000
H	1.68300000	3.01100000	-0.21000000
H	-0.05100000	4.70700000	-0.08300000
H	-2.43900000	4.04200000	0.08800000

### G6cH [+6]

N	-5.44600000	1.74900000	-3.67300000
N	-1.10600000	-0.73100000	-3.68400000
N	1.17800000	-0.18600000	-3.77800000
N	1.18600000	-5.17800000	-3.76400000
C	-5.12300000	0.45300000	-3.55600000
H	-5.93800000	-0.24400000	-3.43100000
C	-3.80700000	0.04500000	-3.58900000
H	-3.57600000	-1.00500000	-3.49500000
C	-2.79400000	0.98600000	-3.73600000
C	-1.36600000	0.57200000	-3.73400000
C	0.18000000	-1.06100000	-3.73200000
C	0.53000000	-2.50500000	-3.74900000
C	-0.42800000	-3.47500000	-3.48100000
H	-1.45000000	-3.19800000	-3.26400000
C	-0.06900000	-4.80400000	-3.48400000
H	-0.77200000	-5.59700000	-3.27200000
C	2.12200000	-4.26200000	-4.05800000
H	3.10500000	-4.63700000	-4.31000000
C	1.82500000	-2.91900000	-4.04900000
H	2.59400000	-2.20200000	-4.29600000
N	-5.21000000	1.26000000	3.37100000
N	-0.87400000	-1.18600000	3.72400000
N	1.41300000	-0.63300000	3.69600000
N	1.33800000	-5.63100000	3.45200000
C	-4.85100000	-0.00900000	3.12800000
H	-5.64000000	-0.68700000	2.83400000

C	-3.53900000	-0.40700000	3.24700000
H	-3.27700000	-1.43700000	3.05100000
C	-2.56500000	0.52300000	3.59000000
C	-1.13800000	0.11600000	3.67300000
C	0.41300000	-1.50900000	3.72100000
C	0.75100000	-2.95500000	3.67800000
C	-0.18600000	-3.92000000	4.03700000
H	-1.16000000	-3.63900000	4.41300000
C	0.13900000	-5.25100000	3.92400000
H	-0.54500000	-6.04100000	4.20800000
C	2.26200000	-4.71800000	3.12000000
H	3.20900000	-5.09700000	2.76200000
C	2.00000000	-3.37300000	3.23600000
H	2.76100000	-2.65400000	2.96500000
N	-0.43700000	1.52400000	-3.78900000
N	3.96300000	3.94500000	-3.77500000
C	-4.48500000	2.67200000	-3.84900000
H	-4.81600000	3.69600000	-3.96700000
C	-3.15500000	2.32100000	-3.88100000
H	-2.40600000	3.08800000	-4.01700000
C	0.82200000	1.09500000	-3.79600000
C	1.91600000	2.10100000	-3.82300000
C	1.66000000	3.45600000	-4.02100000
H	0.65500000	3.81200000	-4.19800000
C	2.70400000	4.35300000	-4.00100000
H	2.56200000	5.41300000	-4.16900000
C	4.23500000	2.64500000	-3.60600000
H	5.27200000	2.38500000	-3.44500000
C	3.23300000	1.70100000	-3.63800000
H	3.47900000	0.65900000	-3.50200000
N	-0.21300000	1.07000000	3.64800000
N	4.12000000	3.55500000	3.39000000
C	-4.29000000	2.17200000	3.73000000
H	-4.65200000	3.16800000	3.95000000
C	-2.95900000	1.83700000	3.83100000
H	-2.24000000	2.59100000	4.12000000
C	1.04700000	0.64400000	3.65800000
C	2.12500000	1.66600000	3.57900000
C	1.84800000	2.94900000	3.12300000
H	0.84600000	3.23100000	2.83200000
C	2.86700000	3.87000000	3.02900000
H	2.70400000	4.87900000	2.67600000
C	4.40900000	2.32400000	3.84500000
H	5.43300000	2.14400000	4.14600000
C	3.43400000	1.35700000	3.93800000
H	3.69300000	0.37600000	4.31200000
C	5.94200000	5.48100000	-0.04500000
H	6.61200000	6.30500000	0.14400000
C	5.19600000	5.12000000	-1.14400000
N	4.84000000	3.61300000	0.37500000
N	4.54300000	3.97300000	-0.83300000

N	5.68000000	4.52000000	0.86600000
C	5.00300000	5.82100000	-2.44700000
H	4.05900000	6.37700000	-2.43200000
H	5.78100000	6.57700000	-2.57500000
C	6.20800000	4.34800000	2.20300000
H	6.65200000	3.35300000	2.27000000
C	5.05900000	4.94300000	-3.69500000
H	4.98800000	5.56700000	-4.58700000
H	5.99500000	4.38900000	-3.74800000
C	5.19000000	4.57700000	3.31300000
H	5.71200000	4.57300000	4.27200000
H	4.70400000	5.54700000	3.20600000
H	7.01200000	5.07100000	2.34600000
C	-7.32300000	1.62400000	-1.20900000
N	-6.24900000	1.02800000	0.57500000
N	-6.42500000	0.75700000	-0.67800000
N	-7.02700000	2.06100000	0.87700000
C	-7.76100000	1.51100000	-2.63000000
H	-7.90900000	0.45600000	-2.87100000
H	-8.74400000	1.97100000	-2.75500000
C	-6.87100000	2.18700000	-3.66800000
H	-7.26300000	1.99700000	-4.67000000
H	-6.85200000	3.26500000	-3.51500000
C	-6.64200000	1.64600000	3.30200000
H	-6.89300000	2.09400000	4.26500000
C	1.82000000	-7.82600000	-0.23900000
H	2.10400000	-8.86600000	-0.19800000
C	1.90700000	-6.87800000	-1.23100000
N	0.98700000	-5.91000000	0.47600000
N	1.38800000	-5.72300000	-0.74200000
N	1.25100000	-7.17600000	0.79600000
C	2.49100000	-6.98500000	-2.59800000
H	3.40700000	-6.38800000	-2.65900000
H	2.80200000	-8.01600000	-2.78100000
C	1.55800000	-6.61400000	-3.74800000
H	2.04200000	-6.82800000	-4.70300000
H	0.63100000	-7.18300000	-3.70800000
C	1.62300000	-7.07000000	3.26200000
H	1.34200000	-7.58900000	4.18000000
C	-7.72100000	2.47500000	-0.20200000
H	-8.43300000	3.28500000	-0.16800000
H	2.70000000	-7.17700000	3.13500000
C	0.86400000	-7.68800000	2.09400000
H	1.06100000	-8.76100000	2.10800000
H	-0.21300000	-7.55600000	2.21200000
H	-7.22000000	0.72900000	3.20000000
C	-6.99800000	2.63800000	2.20900000
H	-7.99700000	3.01600000	2.43500000
H	-6.32100000	3.49700000	2.21600000
C	-1.61500000	0.65800000	0.45200000
C	-0.86400000	-0.53200000	0.51900000

C	-0.71600000	1.73900000	0.39500000
C	0.50000000	-0.18700000	0.49600000
C	0.59100000	1.21600000	0.41600000
C	-2.89500000	0.71200000	-0.04500000
C	-1.34000000	-1.75400000	0.10600000
C	-1.03200000	2.95500000	-0.16100000
C	1.48700000	-1.03500000	0.05200000
C	1.67500000	1.87200000	-0.11500000
C	1.03400000	-2.38200000	-0.17900000
C	-0.30600000	-2.72300000	-0.14600000
C	-2.42600000	3.10100000	-0.48900000
C	-3.30700000	2.03700000	-0.43400000
C	0.11500000	3.74400000	-0.53100000
C	1.39800000	3.23000000	-0.50900000
C	2.71200000	-0.36400000	-0.30300000
C	2.80400000	1.01400000	-0.37700000
C	-3.48300000	-0.58200000	-0.28800000
C	-2.74500000	-1.75000000	-0.21400000
H	1.73500000	-3.16100000	-0.45900000
H	-2.78900000	4.05300000	-0.86300000
H	-0.56500000	-3.74900000	-0.38700000
H	-4.32400000	2.19600000	-0.77000000
H	-0.03000000	4.75100000	-0.90900000
H	3.58100000	-0.94900000	-0.58800000
H	2.21600000	3.84300000	-0.86600000
H	3.73800000	1.45800000	-0.69700000
H	-4.52100000	-0.63900000	-0.59800000
H	-3.23900000	-2.68100000	-0.47700000

### **G7cH [+6]**

N	-5.54800000	1.11300000	-3.21900000
N	-1.15800000	-1.20800000	-3.69800000
N	1.08200000	-0.57900000	-4.03100000
N	1.30300000	-5.55100000	-3.98000000
C	-5.20800000	-0.13800000	-3.56900000
H	-6.02200000	-0.82900000	-3.75200000
C	-3.88900000	-0.50100000	-3.70200000
H	-3.64200000	-1.51200000	-3.99500000
C	-2.89000000	0.44700000	-3.49100000
C	-1.46000000	0.08600000	-3.66300000
C	0.12800000	-1.48900000	-3.88200000
C	0.53100000	-2.91500000	-3.93100000
C	-0.33200000	-3.91500000	-3.50200000
H	-1.32200000	-3.67300000	-3.14000000
C	0.08600000	-5.22600000	-3.52600000
H	-0.53700000	-6.04300000	-3.19000000
C	2.14100000	-4.60600000	-4.43500000
H	3.09400000	-4.94800000	-4.81800000
C	1.78500000	-3.27900000	-4.41400000
H	2.47400000	-2.53500000	-4.78700000



N	-4.62100000	1.39300000	3.70900000
N	-0.27200000	-0.95600000	3.17600000
N	1.98400000	-0.38700000	2.83600000
N	2.02100000	-5.37700000	3.11900000
C	-4.28400000	0.11700000	3.47100000
H	-5.09300000	-0.60000000	3.43600000
C	-2.97100000	-0.24400000	3.28600000
H	-2.72200000	-1.28000000	3.10700000
C	-1.97800000	0.72800000	3.32200000
C	-0.55500000	0.34200000	3.12500000
C	1.00800000	-1.27000000	3.02100000
C	1.37100000	-2.70800000	3.07000000
C	0.47900000	-3.64700000	3.58100000
H	-0.48100000	-3.34600000	3.97500000
C	0.83400000	-4.97500000	3.60200000
H	0.18700000	-5.74300000	4.00600000
C	2.90200000	-4.48900000	2.63900000
H	3.84100000	-4.88500000	2.27800000
C	2.60900000	-3.14400000	2.61500000
H	3.33500000	-2.44300000	2.23000000
N	-0.57600000	1.07300000	-3.79000000
N	3.70500000	3.61600000	-4.46500000
C	-4.60400000	2.03800000	-3.00400000
H	-4.95000000	3.02600000	-2.73200000
C	-3.26700000	1.73800000	-3.14300000
H	-2.52800000	2.51000000	-2.97900000
C	0.68300000	0.68800000	-3.97800000
C	1.72900000	1.72800000	-4.15300000
C	1.40500000	3.05700000	-4.40300000
H	0.37500000	3.37500000	-4.48700000
C	2.41600000	3.97800000	-4.56600000
H	2.22200000	5.01900000	-4.79000000
C	4.03800000	2.34100000	-4.22700000
H	5.09400000	2.12100000	-4.16100000
C	3.07100000	1.37400000	-4.08100000
H	3.36200000	0.34900000	-3.90300000
N	0.34400000	1.30200000	2.93300000
N	4.62700000	3.82900000	2.39300000
C	-3.67900000	2.34700000	3.77100000
H	-4.01600000	3.35100000	3.99400000
C	-2.35000000	2.04600000	3.56900000
H	-1.61200000	2.83400000	3.62200000
C	1.60200000	0.88600000	2.80100000
C	2.66100000	1.91400000	2.63400000
C	2.34200000	3.21900000	2.27900000
H	1.31800000	3.51300000	2.09400000
C	3.34700000	4.15300000	2.15900000
H	3.14800000	5.18000000	1.88600000
C	4.96000000	2.57400000	2.74000000
H	6.00700000	2.38300000	2.93500000
C	4.00000000	1.59700000	2.85900000

H	4.29200000	0.59800000	3.15100000
C	5.99900000	5.59400000	-1.10600000
H	6.46700000	6.55800000	-0.98300000
C	5.29500000	5.02400000	-2.14300000
N	5.42700000	3.52600000	-0.58100000
N	4.97500000	3.76100000	-1.77100000
N	6.04500000	4.62800000	-0.16600000
C	4.86700000	5.61300000	-3.44800000
H	3.91200000	6.13600000	-3.33000000
H	5.58000000	6.38300000	-3.75300000
C	6.66200000	4.63300000	1.14200000
H	7.19800000	3.69000000	1.25900000
C	4.77400000	4.63700000	-4.61300000
H	4.56400000	5.18300000	-5.53400000
H	5.70900000	4.09500000	-4.75200000
C	5.68000000	4.86500000	2.28400000
H	6.23000000	4.88000000	3.22800000
H	5.17500000	5.82500000	2.17900000
H	7.40400000	5.43300000	1.17900000
C	-7.07200000	1.19100000	-0.54100000
N	-5.55900000	1.30400000	1.00000000
N	-5.80000000	0.87300000	-0.19600000
N	-6.66300000	1.89000000	1.45400000
C	-7.64500000	0.80300000	-1.86000000
H	-7.61600000	-0.28500000	-1.96500000
H	-8.70100000	1.07800000	-1.90300000
C	-6.98200000	1.46100000	-3.06900000
H	-7.48600000	1.14900000	-3.98500000
H	-7.03900000	2.54700000	-3.01000000
C	-6.05200000	1.74500000	3.87100000
H	-6.14900000	2.31600000	4.79700000
C	2.29300000	-7.84800000	-0.38400000
H	2.57900000	-8.88500000	-0.28900000
C	2.31900000	-6.97200000	-1.44200000
N	1.51500000	-5.88100000	0.25000000
N	1.83800000	-5.78000000	-1.00100000
N	1.79600000	-7.12600000	0.63900000
C	2.80400000	-7.18500000	-2.83500000
H	3.67900000	-6.55500000	-3.02300000
H	3.15100000	-8.21500000	-2.94700000
C	1.76500000	-6.95700000	-3.93100000
H	2.19000000	-7.19500000	-4.90700000
H	0.88500000	-7.58100000	-3.78500000
C	2.32300000	-6.82200000	3.05400000
H	2.10300000	-7.25600000	4.03200000
C	-7.64000000	1.85300000	0.52500000
H	-8.62200000	2.27200000	0.68500000
H	3.39200000	-6.92800000	2.87300000
C	1.50500000	-7.54800000	1.99300000
H	1.73100000	-8.61200000	2.07300000
H	0.43500000	-7.43000000	2.17300000

H	-6.60100000	0.81300000	3.99600000
C	-6.63200000	2.57300000	2.73300000
H	-7.65700000	2.82500000	3.01000000
H	-6.09000000	3.51600000	2.61800000
C	-1.74100000	-2.03800000	-0.12000000
C	-0.44500000	-2.46100000	-0.25700000
C	0.59200000	-1.51900000	-0.42800000
C	0.28600000	-0.12700000	-0.42900000
C	-1.06200000	0.29300000	-0.24300000
C	-2.04800000	-0.67200000	-0.11900000
H	2.13900000	-3.00400000	-0.62700000
H	-2.54200000	-2.76100000	-0.01000000
H	-0.19200000	-3.51600000	-0.24500000
C	1.92800000	-1.94000000	-0.60200000
C	1.33300000	0.82000000	-0.61900000
H	-3.08600000	-0.37900000	-0.02200000
C	2.63200000	0.35600000	-0.74600000
C	2.92700000	-1.01200000	-0.74400000
H	3.45100000	1.05700000	-0.85500000
H	3.95600000	-1.33200000	-0.86500000
C	-2.63100000	2.19400000	0.09000000
C	-1.36300000	1.72600000	-0.18900000
C	-0.32800000	2.66700000	-0.43600000
C	-0.63500000	4.05800000	-0.43900000
C	-1.95200000	4.48400000	-0.16500000
C	-2.92600000	3.56100000	0.10500000
H	-3.43300000	1.50500000	0.30300000
C	1.00600000	2.24600000	-0.68300000
C	0.38200000	4.99600000	-0.72000000
H	-2.17400000	5.54500000	-0.16800000
H	-3.93800000	3.88400000	0.32300000
C	1.65200000	4.56600000	-0.99400000
C	1.95900000	3.20000000	-0.97500000
H	0.13600000	6.05200000	-0.72400000
H	2.43400000	5.28100000	-1.22500000
H	2.97500000	2.91400000	-1.20400000