

Supporting Information

Recognition and electrochemiluminescence response of benzo[6]urils to polycyclic aromatic hydrocarbons

Hai-Ling Li, Fang Wang, Qing-Mei Ge, Fei Qiu, Hang Cong*, Zhu Tao

Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang 550025, China. E-mail: hcong@gzu.edu.cn

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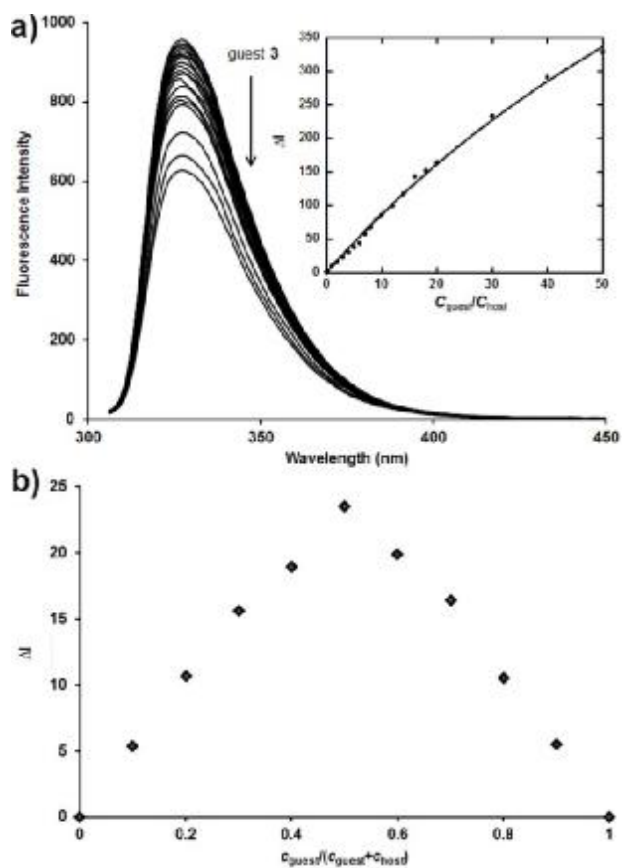


Figure S1. a) Fluorescence titration spectra of benzo[6]uril **1** with guest **3**. The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$ in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ (5:1, v/v). Inset: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$). b) Job's plots of the interaction between benzo[6]uril **1** and a) guest **3**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$.

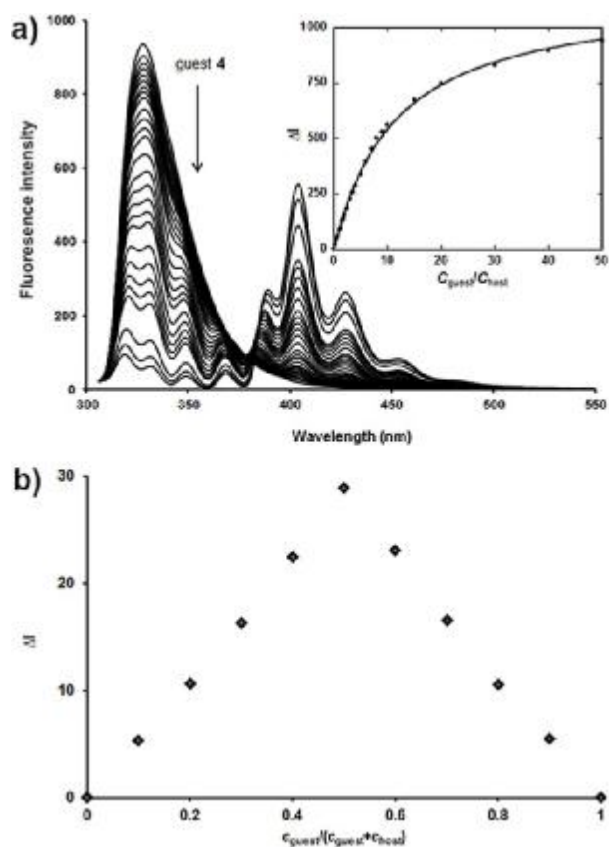


Figure S2. a) Fluorescence titration spectra of benzo[6]uril **1** with guest **4**. The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$ in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ (5:1, v/v). Inset: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$). b) Job's plots of the interaction between benzo[6]uril **1** and a) guest **4**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$.

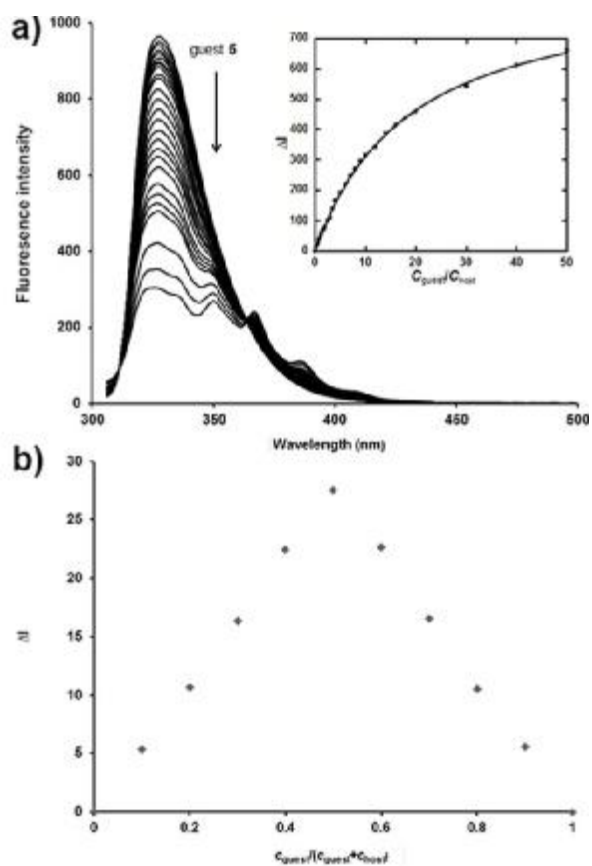


Figure S3. a) Fluorescence titration spectra of benzo[6]uril **1** with guest **5**. The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$ in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ (5:1, v/v). Inset: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$). b) Job's plots of the interaction between benzo[6]uril **1** and a) guest **5**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$.

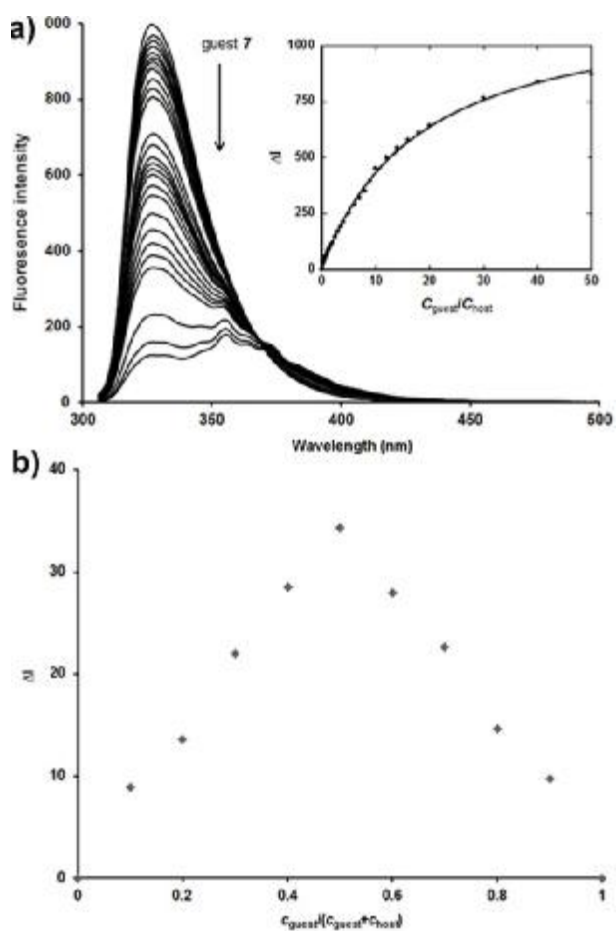


Figure S4. a) Fluorescence titration spectra of benzo[6]uril **1** with guest **7**. The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$ in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ (5:1, v/v). Inset: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$). b) Job's plots of the interaction between benzo[6]uril **1** and a) guest **7**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$.

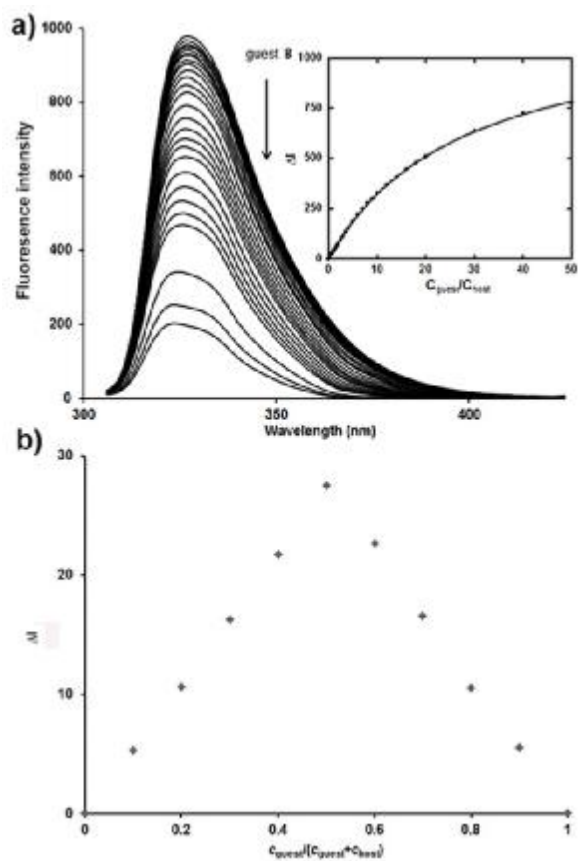


Figure S5. a) Fluorescence titration spectra of benzo[6]uril **1** with guest **8**. The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$ in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ (5:1, v/v). Inset: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$). b) Job's plots of the interaction between benzo[6]uril **1** and a) guest **8**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{\text{em}} = 327 \text{ nm}$, $\lambda_{\text{ex}} = 304 \text{ nm}$.

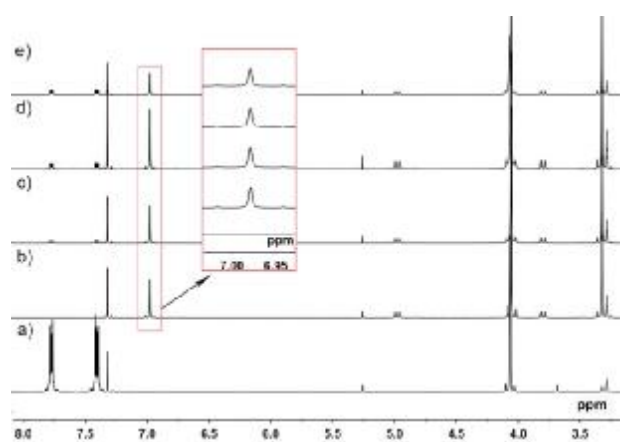


Figure S6. ¹H NMR spectra (400 MHz, CD₃Cl/CD₃OD, 5:1,v/v) of (a) free guest **3**; (b) free benzo[6]uril **1** ($2.0 \times 10^{-3} \text{ mol} \cdot \text{L}^{-1}$), and in the presence of (c) 0.5 equiv ; (d) 1 equiv ; (e) 2 equiv of guest **3**.

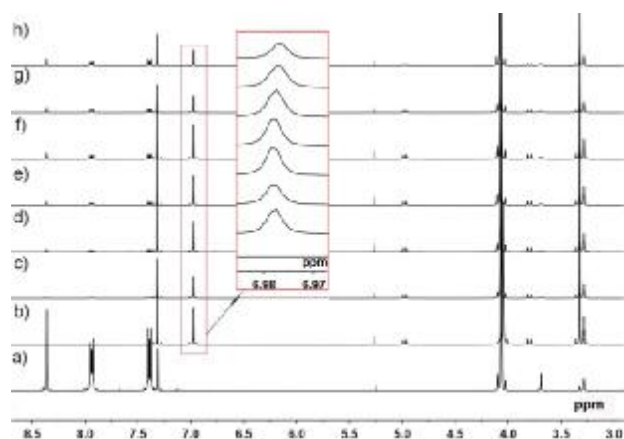


Figure S7. ^1H NMR spectra (400 MHz, $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$, 5:1, v/v) of (b) free benzo[6]juril **1** ($2.0 \times 10^{-3} \text{ mol} \cdot \text{L}^{-1}$), and in the presence of (c) 0.25 equiv ; (d) 0.5 equiv ; (e) 0.75 equiv ; (f) 1 equiv ; (g) 1.5 equiv ; (h) 2 equiv of guest **4**, and (a) free guest **4**.

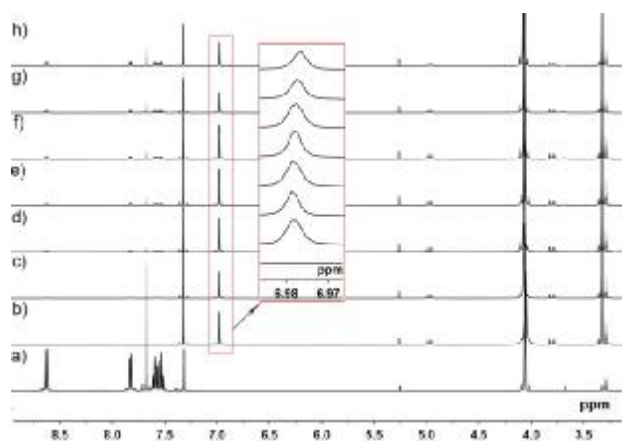


Figure S8. ^1H NMR spectra (400 MHz, $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$, 5:1,v/v) of (b) free benzo[6]juril **1** ($2.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$), and in the presence of (c) 0.25 equiv ; (d) 0.5 equiv ; (e) 0.75 equiv ; (f) 1 equiv ; (g) 1.5 equiv ; (h) 2 equiv of guest **5**, and (a) free guest **5**.

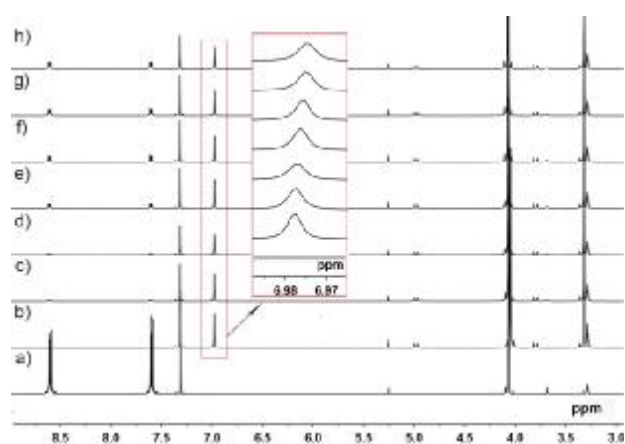


Figure S9. ^1H NMR spectra (400 MHz, $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$, 5:1,v/v) of (b) free benzo[6]juril **1** ($2.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$), and in the presence of (c) 0.25 equiv ; (d) 0.5 equiv ; (e) 0.75 equiv ; (f) 1 equiv ; (g) 2 equiv ; (h) 3 equiv of guest **7**, and (a) free guest **7**.

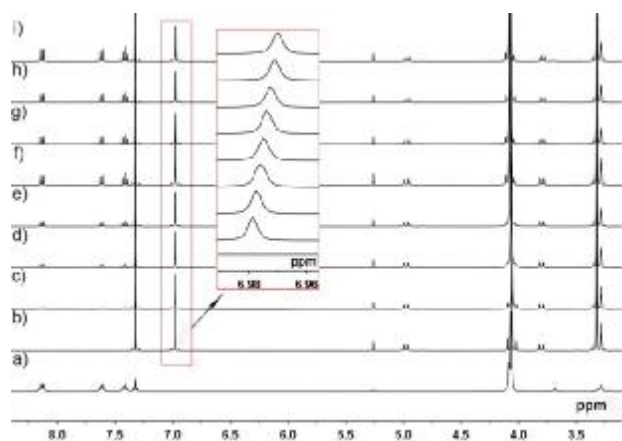


Figure S10. ^1H NMR spectra (400 MHz, $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$, 5:1, v/v) of (b) free benzo[6]juril **1** ($2.0 \times 10^{-3} \text{ mol} \cdot \text{L}^{-1}$), and in the presence of (c) 0.25 equiv ; (d) 0.5 equiv ; (e) 0.75 equiv ; (f) 1 equiv ; (g) 1.5 equiv ; (h) 2 equiv of guest **8**, and (a) free guest **8**.

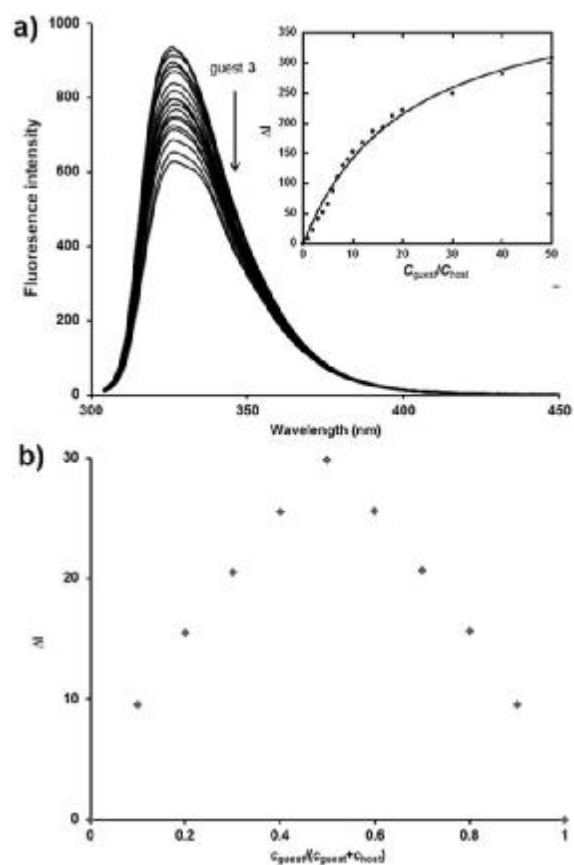


Figure S11. Fluorescence titration spectra of benzo[6]juril **2** with guest **3**. **a)** The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$ in DMSO. Inset: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{\text{em}} = 326 \text{ nm}$, $\lambda_{\text{ex}} = 300 \text{ nm}$). **b)** Job's plots of the interaction between benzo[6]juril **2** and a) guest **3**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{\text{em}} = 326 \text{ nm}$, $\lambda_{\text{ex}} = 300 \text{ nm}$.

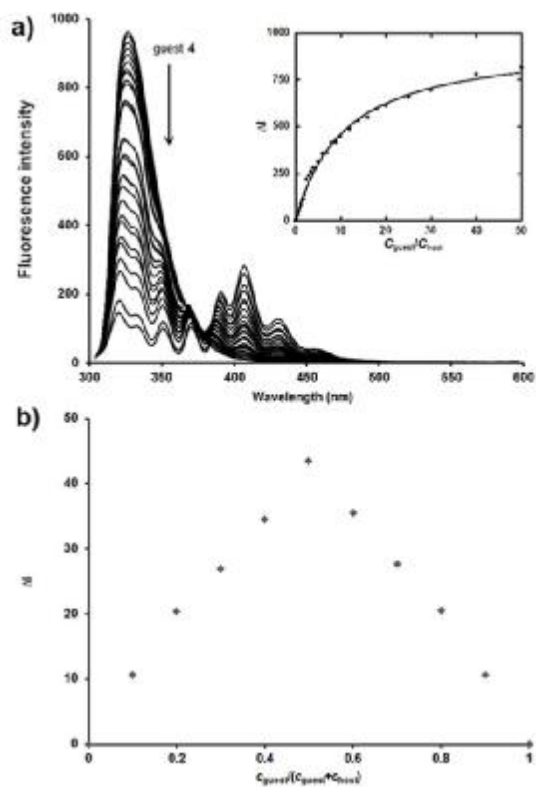


Figure S12. Fluorescence titration spectra of benzo[6]uril **2** with guest **4**. **a)** The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$ in DMSO. Insets: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{em} = 326 \text{ nm}$, $\lambda_{ex} = 300 \text{ nm}$). **b)** Job's plots of the interaction between benzo[6]uril **2** and a) guest **4**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{em} = 326 \text{ nm}$, $\lambda_{ex} = 300 \text{ nm}$.

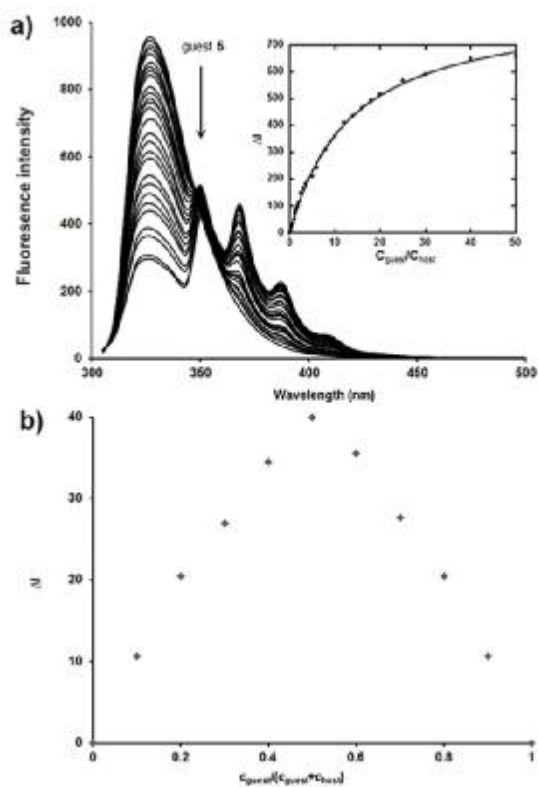


Figure S13. Fluorescence titration spectra of benzo[6]juril **2** with guest **5**. **a)** The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$ in DMSO. Insets: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{em} = 326 \text{ nm}$, $\lambda_{ex} = 300 \text{ nm}$). **b)** Job's plots of the interaction between benzo[6]juril **2** and **a)** guest **5**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{em} = 326 \text{ nm}$, $\lambda_{ex} = 300 \text{ nm}$.

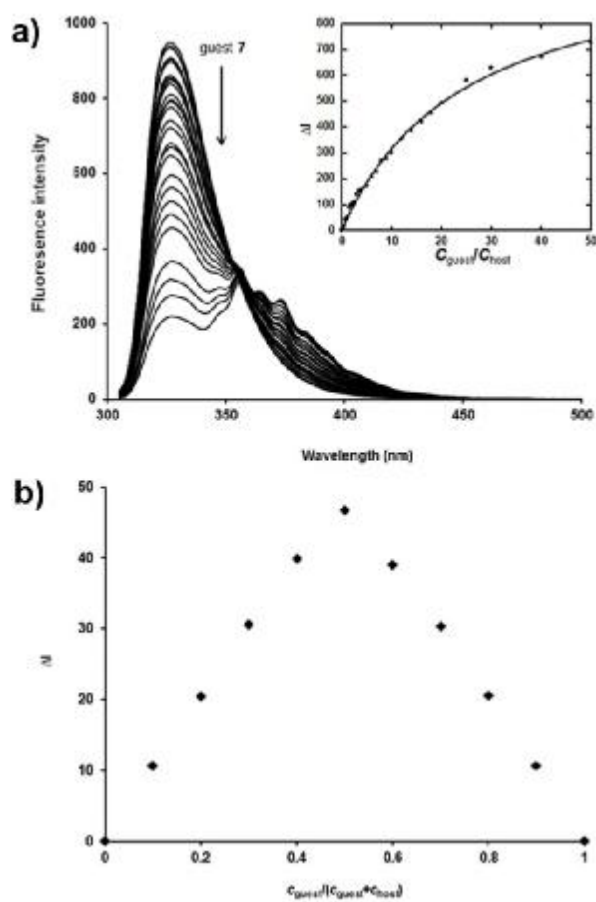


Figure S14. Fluorescence titration spectra of benzo[6]uril **2** with guest **7**. **a)** The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$ in DMSO. Insets: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{\text{em}} = 326 \text{ nm}$, $\lambda_{\text{ex}} = 300 \text{ nm}$). **b)** Job's plots of the interaction between benzo[6]uril **2** and a) guest **7**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{\text{em}} = 326 \text{ nm}$, $\lambda_{\text{ex}} = 300 \text{ nm}$.

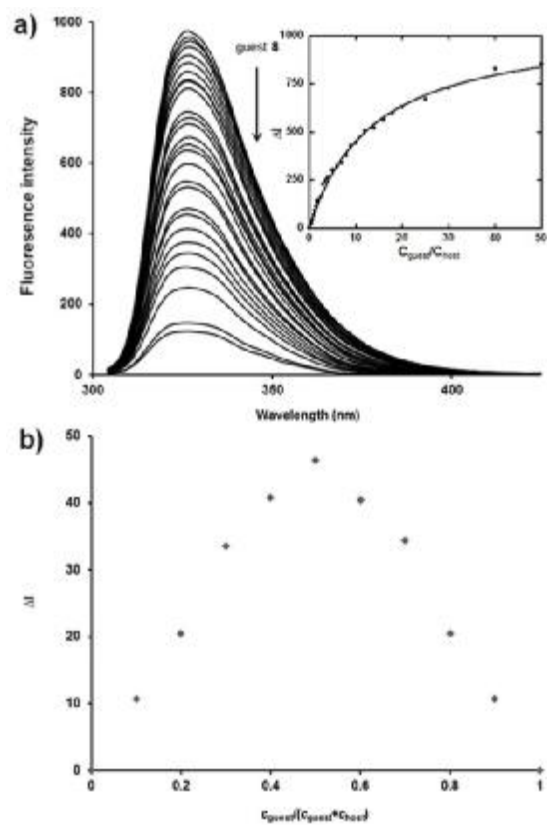


Figure S15. Fluorescence titration spectra of benzo[6]juril **2** with guest **8**. **a)** The host concentration was fixed at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$ in DMSO. Inset: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{\text{em}} = 326 \text{ nm}$, $\lambda_{\text{ex}} = 300 \text{ nm}$). **b)** Job's plots of the interaction between benzo[6]juril **2** and a) guest **8**. The total concentration was maintained at $1.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$, and fluorescence intensities were recorded at $\lambda_{\text{em}} = 326 \text{ nm}$, $\lambda_{\text{ex}} = 300 \text{ nm}$.

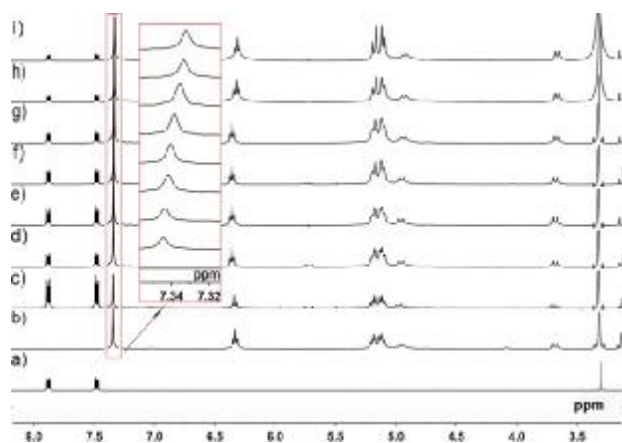


Figure S16. ^1H NMR spectra (400 MHz, $[\text{D}_6]\text{DMSO}$) of (b) free benzo[6]juril **2** ($2.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$), and in the presence of (c) 0.5 equiv; (d) 1 equiv; (e) 1.5 equiv; (f) 2 equiv; (g) 2.5 equiv; (h) 3 equiv; (i) 3.5 equiv of guest **3**, and (a) free guest **3**.

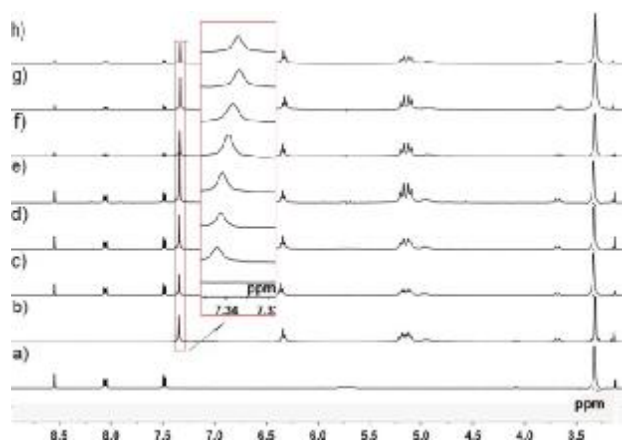


Figure S17. ^1H NMR spectra (400 MHz, $[\text{D}_6]\text{DMSO}$) of (b) free benzo[6]juril **2** ($2.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$), and in the presence of (c) 0.5 equiv; (d) 1 equiv; (e) 1.5 equiv; (f) 2 equiv; (g) 2.5 equiv; (h) 2.5 equiv; (i) 3 equiv of guest **4**, and (a) free guest **4**.

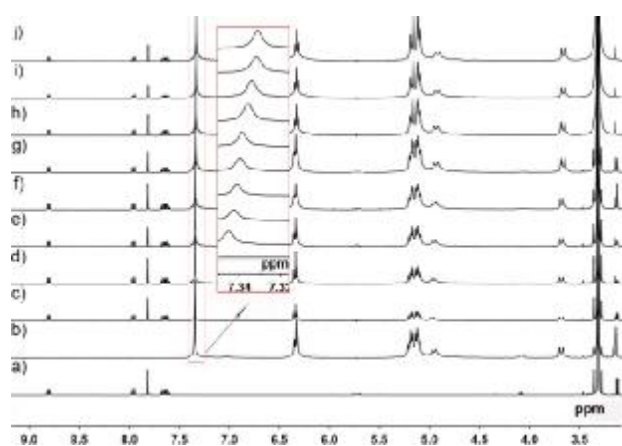


Figure S18. ^1H NMR spectra (400 MHz, $[\text{D}_6]\text{DMSO}$) of (b) free benzo[6]juril **2** ($2.0 \times 10^{-3} \text{ mol} \cdot \text{L}^{-1}$), and in the presence of (c) 0.25 equiv; (d) 0.5 equiv; (e) 0.75 equiv; (f) 1 equiv; (g) 1.5 equiv; (h) 2 equiv; (i) 2.5 equiv; (j) 3 equiv of guest **5**, and (a) free guest **5**.

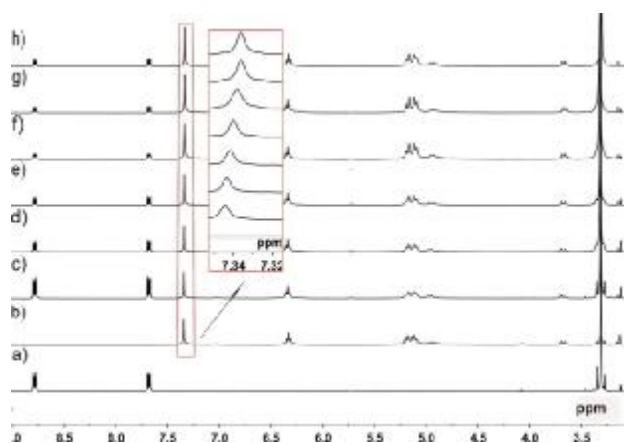


Figure S19. ^1H NMR spectra (400 MHz, $[\text{D}_6]\text{DMSO}$) of (b) free benzo[6]juril **2** ($2.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$), and in the presence of (c) 0.5 equiv; (d) 1 equiv; (e) 1.5 equiv; (f) 2 equiv; (g) 2.5 equiv; (h) 3 equiv of guest **7**, and (a) free guest **7**.

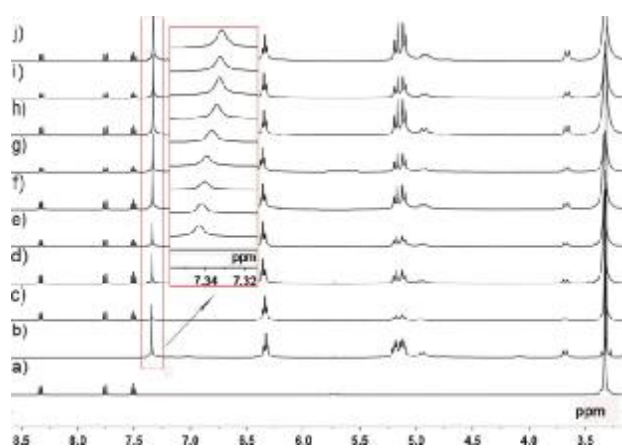


Figure S20. ^1H NMR spectra (400 MHz, $[\text{D}_6]\text{DMSO}$) of (b) free benzo[6]juril **2** ($2.0 \times 10^{-3} \text{ mol} \cdot \text{L}^{-1}$), and in the presence of (c) 0.25 equiv; (d) 0.5 equiv; (e) 0.75 equiv; (f) 1 equiv; (g) 1.5 equiv; (h) 2 equiv; (i) 2.5 equiv; (j) 3 equiv of guest **8**, and (a) free guest **8**.

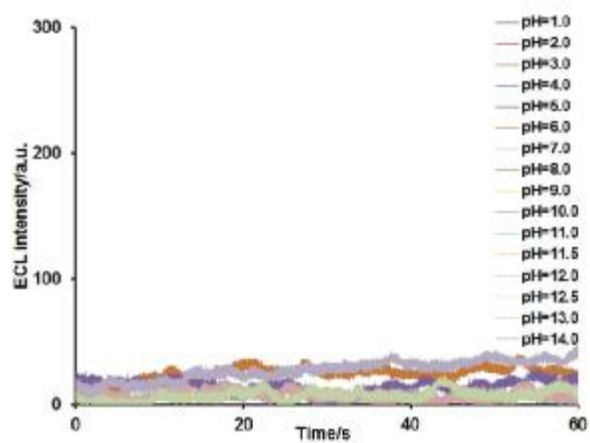


Figure S21. The ECL blank test in the PBS solution at different pH values.

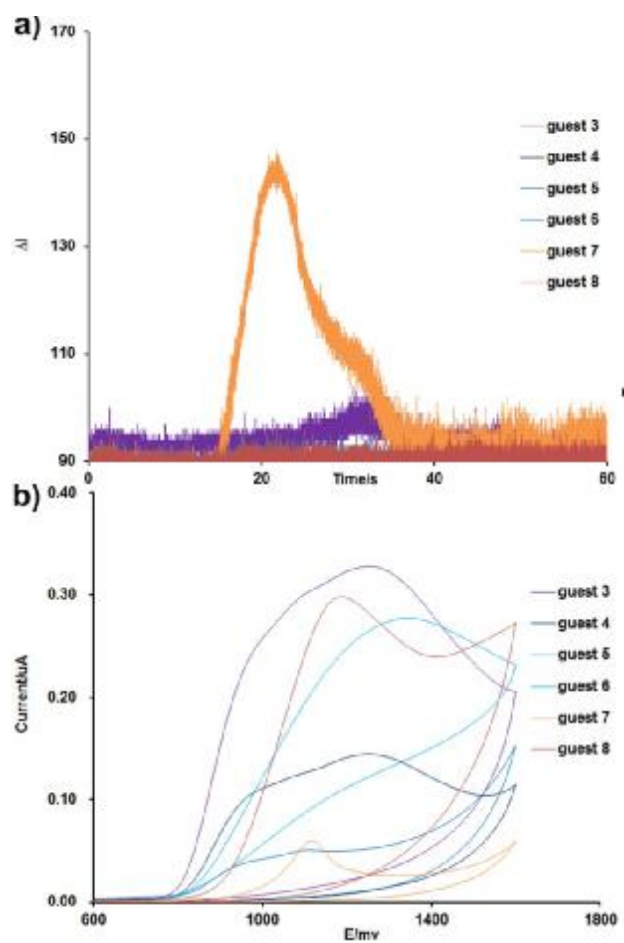


Figure S22. a) All guests on ECL intensity of benzo[6]uril 1/GCE; b) All guests on currents of benzo[6]uril 1/GCE;

Coordinates of the optimized structures

1. Guest 3@benzo[6]uril 1

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	-1.73793000	0.18884500	3.66988100
C	0.01364700	0.16603900	2.00478000
C	-0.52049200	-0.07226900	-0.36549000
C	1.77465800	0.12074100	0.34877900
C	1.38552700	0.21176900	1.65536200
C	0.81112500	-0.02129100	-0.67487100
C	-2.70845600	0.02755800	2.65386900
C	-0.95704700	0.01326600	0.98156000
C	-2.32726800	-0.05730100	1.34122700
C	-0.40870600	0.25146700	3.35523600
H	-2.05675400	0.25195800	4.70421400
H	-1.26376800	-0.17133900	-1.14900600
H	2.82520400	0.15415100	0.09203900
H	2.11851900	0.29371800	2.45033000
H	1.13193600	-0.08612400	-1.70905200
H	-3.75623200	-0.02207500	2.92753100
H	-3.06529500	-0.19074100	0.55700000
H	0.34705900	0.33841200	4.12786100
C	6.13049800	-2.04405400	-1.17760800
C	4.83344200	-2.51715800	-1.35740400
C	3.90915700	-1.59757000	-1.84891500
C	4.23162200	-0.26178100	-2.04060400
C	5.49946400	0.24479700	-1.75887500
C	6.46060300	-0.69204500	-1.38930300
N	7.28601000	-2.67575500	-0.72072000
C	8.33186500	-1.77057400	-0.67404000
N	7.80642300	-0.54703000	-1.05700800
O	9.48416600	-2.00434800	-0.37936700
C	4.15920200	2.60485000	0.03472000
C	3.04494500	3.37308100	0.42820300
C	4.58195800	2.56579300	-1.29227100
C	3.84588300	3.33858700	-2.19353200
C	2.78607700	4.13680000	-1.79241900
C	2.37051600	4.19847200	-0.46210800
N	4.62592900	1.96878000	1.18270800
C	3.81532800	2.28569500	2.26098700
N	2.85500200	3.15803700	1.78803000
O	3.92025300	1.86078700	3.39352500
C	1.32610700	5.20965900	-0.05377000

C	-1.12869900	5.79916100	-0.36547200
C	-0.11756100	4.83837900	-0.33240900
C	-0.50723000	3.52738300	-0.59177600
C	-1.81839200	3.20126300	-0.92316000
C	-2.82150600	4.16190200	-1.01988400
C	-2.45083400	5.46996600	-0.70744400
N	-1.10196100	7.17363200	-0.13030500
C	-2.36597400	7.70747100	-0.30628700
N	-3.18390100	6.65577900	-0.68081900
O	-2.69484800	8.86538800	-0.15212300
C	-4.22073600	3.81970800	-1.50070000
C	-5.00638400	1.58884700	-0.53472400
C	-4.54154600	2.35085100	-1.60246600
C	-4.41474900	1.68931900	-2.82257900
C	-4.74545500	0.34944800	-2.97192600
C	-5.23345800	-0.41655200	-1.91386800
C	-5.36495900	0.23650400	-0.69078400
N	-5.23300000	1.91932500	0.79577400
C	-5.73069000	0.82343900	1.47330900
N	-5.80586400	-0.20669400	0.55209700
O	-6.02252700	0.76474700	2.65137000
C	-5.53125000	-1.88295800	-2.11255900
C	-4.68740500	-4.06138800	-1.03757900
C	-4.44539600	-2.79324600	-1.56109200
C	-3.11792400	-2.37210600	-1.54456800
C	-2.09381600	-3.14936300	-1.02342700
C	-2.32961900	-4.40457600	-0.46986000
C	-3.65467700	-4.83908800	-0.48081400
N	-5.86609400	-4.79181200	-0.89471800
C	-5.60063900	-5.99967400	-0.27105100
N	-4.24258300	-6.01157500	-0.00921800
O	-6.40073500	-6.87396100	-0.01318400
C	0.94402500	-3.97149300	0.69478400
C	0.19495500	-4.74946600	-0.18142300
C	0.83108500	-5.13493700	-1.36180300
C	2.15685800	-4.82384400	-1.61649800
C	2.94360400	-4.11723000	-0.70481400
C	2.30250200	-3.67741500	0.45138300
N	0.62021800	-3.41426100	1.92457100
C	1.73367200	-2.80687100	2.47427700
N	2.76333100	-2.97688200	1.56059100
O	1.79884900	-2.23400100	3.54131600
C	4.41563500	-3.92697200	-0.98477200
C	7.53534700	-4.08116600	-0.47969100

C	8.69198000	0.57669100	-1.27397700
C	5.81806300	1.17581900	1.38763800
C	1.69501300	3.47873600	2.59501700
C	-0.02695800	8.01649800	0.34816300
C	-4.60277600	6.87564000	-0.85538900
C	-4.87001800	3.12409800	1.51328900
C	-6.28836500	-1.51005300	0.95481900
C	-7.18475700	-4.53328500	-1.43002900
C	-3.64712700	-7.13790100	0.67719400
C	-0.68176500	-3.27552600	2.54338300
C	4.03706500	-2.32750000	1.78123200
C	-1.20269800	-5.24754600	0.09723300
C	5.75066200	1.74222100	-1.78745600
H	2.88807700	-1.92390600	-2.00955700
H	3.45594300	0.43133300	-2.34738200
H	4.13539900	3.32948900	-3.23908000
H	2.27467100	4.75316900	-2.52434800
H	1.55791800	6.12627100	-0.59964900
H	1.45006600	5.46069000	1.00084800
H	0.23601100	2.73821000	-0.56259900
H	-2.06055200	2.16655700	-1.13102600
H	-4.35735200	4.25753700	-2.49489900
H	-4.96241500	4.30102600	-0.86450000
H	-4.05272300	2.24672300	-3.67986500
H	-4.62488700	-0.12290600	-3.94103800
H	-5.65050800	-2.06633000	-3.18518900
H	-6.49043800	-2.12362400	-1.66008700
H	-2.88468300	-1.39353000	-1.94558000
H	-1.08119300	-2.76380600	-1.03924300
H	0.27390600	-5.72536900	-2.08161800
H	2.61614800	-5.17261100	-2.53534300
H	4.98100900	-4.25094800	-0.11059700
H	4.69312200	-4.61621600	-1.78839000
H	7.15549900	-4.68745600	-1.30291500
H	8.61615000	-4.20077400	-0.41086000
H	7.08988000	-4.41751400	0.45910600
H	8.52015500	1.01706600	-2.25734600
H	8.57619900	1.34305500	-0.50347200
H	9.70946500	0.19011400	-1.22070700
H	6.71272900	1.72643100	1.08877300
H	5.87273200	0.96793100	2.45555000
H	5.77031600	0.23373100	0.84327000
H	0.77865500	3.30772800	2.02675300
H	1.70998000	2.81146600	3.45614200

H	1.72607800	4.50887100	2.95748300
H	0.73462800	8.17719100	-0.41755800
H	-0.47578500	8.97725400	0.59806500
H	0.43403400	7.59170200	1.24057800
H	-4.75951500	7.95119600	-0.78122100
H	-4.94315800	6.53015400	-1.83194200
H	-5.18157600	6.38416500	-0.06891000
H	-5.54377800	3.95063100	1.27464600
H	-4.96285900	2.89811800	2.57465200
H	-3.84003600	3.40419900	1.28871400
H	-5.54810000	-2.28207100	0.74457300
H	-6.46047100	-1.45796700	2.02906200
H	-7.23322500	-1.75129400	0.46206600
H	-7.12719400	-4.25921700	-2.48473200
H	-7.74987300	-5.45916800	-1.32693600
H	-7.70430700	-3.74946900	-0.87364100
H	-4.46824800	-7.79143900	0.96971800
H	-2.97238200	-7.69600500	0.02534500
H	-3.11141600	-6.81531400	1.57058500
H	-1.00708200	-4.20643400	3.01470900
H	-0.59177500	-2.50943200	3.31194000
H	-1.41851700	-2.95089400	1.80635200
H	4.85507900	-3.04960100	1.82084700
H	4.23613300	-1.59237400	1.00030600
H	3.96600900	-1.82135500	2.74363200
H	-1.26987700	-6.25162300	-0.32751300
H	-1.34278100	-5.37262700	1.17199500
H	5.97895900	2.05908800	-2.80997000
H	6.63229100	1.98310500	-1.19711200

Total energy: -3816.7983176 a.u.

BSSE corrected energy: -3816.8308357 a.u.

2. Guest 4@benzo[6]juril 1

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	-0.14471000	0.45964700	2.84872100
C	0.40803000	0.18009700	0.49922300
C	-1.37033200	-0.08571600	-1.17627500
C	0.94948200	-0.07404000	-1.84954700
C	1.35948200	0.09496200	-0.56300700
C	-0.43740300	-0.16699000	-2.16124300
C	-1.53928200	0.37114100	2.53757600
C	-0.98553900	0.08919700	0.18560500
C	-1.92430000	0.17758500	1.21027600
C	0.79406800	0.35392500	1.82440500
C	-2.49004900	0.47282600	3.60092900
C	-2.06930400	0.65664700	4.88193600
C	-0.68071900	0.74696400	5.18975700
C	0.25452200	0.64677500	4.20748700
H	-2.42880600	-0.13739100	-1.40411400
H	1.67308800	-0.13150500	-2.65413700
H	2.41434800	0.17741300	-0.32223000
H	-0.74448900	-0.29469800	-3.19402100
H	-2.97633100	0.08326100	0.96693400
H	1.84633700	0.38928600	2.08024900
H	-3.54888700	0.40226100	3.37238100
H	-2.79774900	0.73368400	5.68155100
H	-0.37331200	0.89058400	6.21952900
H	1.31460100	0.71161300	4.42311600
C	6.40089900	-1.73249300	-1.07115100
C	5.17440400	-2.27344500	-1.44225500
C	4.25543500	-1.38505000	-1.99571000
C	4.50184100	-0.02273200	-2.06497100
C	5.68199600	0.54521800	-1.58777300
C	6.65137300	-0.34878200	-1.14174500
N	7.53037800	-2.32058600	-0.50478800
C	8.48983900	-1.35429200	-0.25450500
N	7.92587900	-0.14173400	-0.61655400
O	9.60905600	-1.53487600	0.17400800
C	3.89253700	2.80584900	-0.02504600
C	2.69521000	3.52065500	0.17228000
C	4.53757800	2.78900100	-1.25952600
C	3.91881900	3.50636000	-2.28438700
C	2.76198100	4.24314100	-2.07643700
C	2.13286100	4.30004700	-0.83317700

N	4.20753800	2.21157900	1.19483700
C	3.25018600	2.54567700	2.14220800
N	2.31874800	3.33381400	1.49695400
O	3.23607700	2.19708500	3.30521900
C	0.99915600	5.27096700	-0.60841500
C	-1.52529200	5.56862500	-0.61476000
C	-0.40927000	4.76594400	-0.85488500
C	-0.66052800	3.51754700	-1.41708400
C	-1.94673900	3.11394300	-1.75217400
C	-3.06382900	3.91672000	-1.54688100
C	-2.82370800	5.16376400	-0.97236900
N	-1.63742100	6.84514900	-0.06288000
C	-2.96101700	7.24696300	-0.06637000
N	-3.68171200	6.20865000	-0.63065700
O	-3.40405300	8.30088900	0.34000700
C	-4.44453100	3.43850000	-1.96143300
C	-4.95677800	1.21550200	-0.80086300
C	-4.64354200	1.94090800	-1.94799100
C	-4.57594300	1.21019600	-3.13243500
C	-4.83177200	-0.15463600	-3.17493800
C	-5.18496700	-0.88435900	-2.03988400
C	-5.24424000	-0.16346400	-0.84704400
N	-5.10376900	1.61940700	0.52251700
C	-5.48770000	0.54333700	1.29963600
N	-5.56517300	-0.54633800	0.45182700
O	-5.69104400	0.54512800	2.49788600
C	-5.44666700	-2.37152400	-2.15121300
C	-4.39826200	-4.38340400	-0.92716600
C	-4.27465400	-3.22426400	-1.68981700
C	-2.97242700	-2.83606200	-1.99408400
C	-1.85899100	-3.50900000	-1.51452900
C	-1.97236900	-4.62808400	-0.69430100
C	-3.27065600	-5.05123400	-0.41299400
N	-5.52144500	-5.07430300	-0.47219700
C	-5.12830600	-6.15445200	0.30242900
N	-3.74681200	-6.11906600	0.34740000
O	-5.85509400	-6.97328000	0.82387900
C	1.26328100	-3.88790400	0.38490500
C	0.59367700	-4.74695400	-0.48094300
C	1.28473500	-5.11992900	-1.63344100
C	2.59555900	-4.72997400	-1.86192800
C	3.31168200	-3.95435300	-0.94892700
C	2.60616500	-3.51355200	0.17036700
N	0.87055500	-3.33647500	1.59780400

C	1.93108100	-2.65795000	2.16818900
N	2.99001900	-2.76279000	1.27755800
O	1.93971700	-2.07736600	3.23211700
C	4.78774700	-3.71400500	-1.17393500
C	7.86787300	-3.72327400	-0.38075800
C	8.73066600	1.06074900	-0.60493000
C	5.43088100	1.55921900	1.60916700
C	1.08017900	3.71153800	2.14788300
C	-0.63622200	7.66967900	0.57838600
C	-5.09542300	6.37166100	-0.88691400
C	-4.69099300	2.85987000	1.14933600
C	-5.95065400	-1.84124600	0.96811700
C	-6.89969700	-4.96297800	-0.89744000
C	-3.02267100	-7.08188500	1.14912800
C	-0.46857000	-3.19169600	2.13415100
C	4.20019800	-2.00874100	1.52384700
C	-0.75046900	-5.36693700	-0.18275100
C	5.83228200	2.05474300	-1.52675800
H	3.28788200	-1.76625400	-2.30022100
H	3.72918400	0.64057200	-2.43559300
H	4.38171200	3.51136800	-3.26552500
H	2.34856700	4.82518900	-2.89335300
H	1.17079200	6.11730100	-1.28144100
H	1.08206800	5.68087300	0.39720000
H	0.16589300	2.84072100	-1.60468400
H	-2.08332700	2.13486600	-2.18790600
H	-4.65019800	3.79218500	-2.97718100
H	-5.20649100	3.89352500	-1.33173800
H	-4.33360300	1.73269100	-4.05174200
H	-4.77247500	-0.67356100	-4.12585500
H	-5.67090700	-2.59560200	-3.19887200
H	-6.34465500	-2.62455600	-1.59304400
H	-2.82335200	-1.95469600	-2.60318900
H	-0.87291300	-3.13425700	-1.76176700
H	0.79178100	-5.77278900	-2.34621400
H	3.10236000	-5.07883300	-2.75539300
H	5.32956800	-4.07801400	-0.29996400
H	5.10743100	-4.34840000	-2.00666500
H	7.59751500	-4.26265600	-1.28956400
H	8.94619200	-3.77794700	-0.23341200
H	7.37926700	-4.18591000	0.47967500
H	8.68249300	1.56441700	-1.57165700
H	8.42015500	1.75000900	0.18401000
H	9.75668500	0.75130000	-0.40757600

H	6.27450700	2.25548200	1.59214300
H	5.27403500	1.22584700	2.63428800
H	5.65178900	0.69807200	0.98106500
H	0.22741100	3.44628700	1.52028200
H	1.02325900	3.15466300	3.08172800
H	1.05827000	4.77916900	2.37896600
H	0.17332300	7.92143000	-0.10707800
H	-1.14044800	8.58585400	0.88360700
H	-0.22827100	7.17982400	1.46603000
H	-5.33428600	7.41058200	-0.66135000
H	-5.32788400	6.16671700	-1.93310800
H	-5.70338600	5.73177000	-0.24255700
H	-5.36055000	3.68267700	0.89234300
H	-4.73765600	2.69875100	2.22545900
H	-3.66853700	3.10784400	0.86167900
H	-5.20507100	-2.59565900	0.72129300
H	-6.01627000	-1.73848700	2.05029200
H	-6.92992700	-2.14169700	0.58829100
H	-6.96223200	-4.87444700	-1.98368200
H	-7.40207600	-5.87543200	-0.57736100
H	-7.40457300	-4.11380300	-0.43158300
H	-3.76276700	-7.78109100	1.53659800
H	-2.29521800	-7.63054000	0.55064800
H	-2.51905000	-6.60041300	1.99044900
H	-0.81774200	-4.10961800	2.61309300
H	-0.43045900	-2.40243900	2.88440500
H	-1.16007200	-2.89917000	1.34157400
H	5.08668400	-2.64415900	1.49671200
H	4.31016100	-1.20347900	0.79519400
H	4.09885300	-1.58215200	2.52147200
H	-0.74319400	-6.36701200	-0.62684200
H	-0.83795400	-5.52445300	0.89244400
H	6.24238000	2.42311700	-2.47245800
H	6.55866700	2.32398300	-0.76230300

Total energy: -3970.4170394 a.u.

BSSE corrected energy: -3970.4492852 a.u.

3. Guest 5@benzo[6]juril 1

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	-1.63507300	0.05119000	1.33075000
C	0.78971200	-0.09376700	0.93604600
C	1.55174000	-0.02532500	-1.45450300
C	2.08782000	-0.21928800	1.47087900
C	-1.88147600	0.11665300	0.00685000
C	0.52653800	-0.01695500	-0.49264200
C	-0.80774500	0.09719300	-0.94437300
C	-0.29623600	-0.03323000	1.83578800
C	-0.06506000	-0.06004900	3.22527000
C	-1.06463900	0.20300600	-2.32511900
C	2.29836800	-0.24977800	2.83113600
C	1.21333400	-0.15913700	3.71701600
C	1.27756500	0.06396500	-2.79954700
C	-0.04426500	0.18386500	-3.24447600
H	-2.44163100	0.06357000	2.05409200
H	-2.89625800	0.19039500	-0.36372800
H	-0.91897800	-0.01501100	3.89039800
H	-2.08819900	0.31091000	-2.65520200
H	3.30689200	-0.32690700	3.22101400
H	1.38665600	-0.17809600	4.78682900
H	2.09586600	0.06416400	-3.51214400
H	-0.25865400	0.27018000	-4.30350300
C	3.09891100	-5.06327600	-0.35334400
C	1.86480400	-4.59080200	-0.79974800
C	1.89832400	-3.44449500	-1.58992100
C	3.08837100	-2.80094400	-1.89172100
C	4.32397300	-3.23723000	-1.42197700
C	4.30662500	-4.41577700	-0.68083700
N	3.43718800	-6.17135600	0.42459200
C	4.81018400	-6.24962600	0.56841700
N	5.33662500	-5.15517800	-0.09918900
O	5.43466900	-7.11222900	1.14859500
C	5.34124500	-0.21607700	-0.40275700
C	5.10654500	1.17434100	-0.35952900
C	5.35103700	-0.92165700	-1.60584700
C	5.12292700	-0.16443000	-2.75549000
C	4.91427800	1.20855400	-2.71352800
C	4.90936300	1.92420800	-1.51729900
N	5.54553000	-0.62613400	0.91076500
C	5.44778600	0.45726400	1.76589000

N	5.16693000	1.55527000	0.97616600
O	5.56116600	0.43826100	2.97497400
C	4.75559900	3.42911500	-1.52519100
C	3.08386400	5.15414500	-0.60918000
C	3.35310100	3.93993200	-1.23731400
C	2.24301000	3.19337600	-1.61733800
C	0.93901700	3.60621400	-1.37706900
C	0.66031700	4.80936800	-0.73486700
C	1.76480900	5.56892700	-0.34551200
N	3.92880600	6.14834800	-0.11810600
C	3.18033600	7.17094000	0.43890300
N	1.85432300	6.80272200	0.30183500
O	3.60566200	8.19182200	0.93794600
C	-0.75767500	5.31140300	-0.54632400
C	-2.46281700	3.59685600	0.26907800
C	-1.90520700	4.35054500	-0.75831000
C	-2.59300900	4.32961600	-1.97159400
C	-3.80424400	3.66774300	-2.11947300
C	-4.42612500	3.00052300	-1.06144000
C	-3.71841000	2.97143600	0.13948300
N	-2.02590200	3.38855700	1.57104100
C	-2.96911600	2.65466500	2.26548000
N	-4.01386700	2.42415200	1.38364700
O	-2.89544100	2.26680200	3.41303100
C	-5.79123500	2.37277100	-1.26431000
C	-6.65221500	-0.01920700	-0.84384100
C	-5.74975300	0.86237900	-1.42910000
C	-4.71338100	0.27391800	-2.15352200
C	-4.49454100	-1.09353900	-2.15922100
C	-5.31276900	-1.97368000	-1.45168900
C	-6.43851900	-1.41300200	-0.85812100
N	-7.80588100	0.20688100	-0.09500500
C	-8.34129600	-1.00176300	0.32054400
N	-7.47014300	-1.98667200	-0.11606700
O	-9.38085500	-1.16598500	0.92041400
C	-2.74076600	-3.45396700	0.05751300
C	-3.43597200	-3.68877400	-1.12832800
C	-2.70872000	-4.29559900	-2.15469800
C	-1.40532400	-4.73901300	-1.97922100
C	-0.73082600	-4.58501100	-0.76813100
C	-1.40319200	-3.86946600	0.21770900
N	-3.13773800	-2.91829900	1.27863600
C	-2.07727400	-2.94376600	2.17329300
N	-1.02006600	-3.53790100	1.51069800

O	-2.08066900	-2.51645000	3.30849900
C	0.56600400	-5.32019000	-0.51646400
C	2.58957200	-7.15765700	1.05887100
C	6.76026900	-5.08663400	-0.34858100
C	5.78002100	-1.95007900	1.44309300
C	4.80562900	2.81721100	1.58853100
C	5.35774600	6.30738900	-0.27385000
C	0.81552600	7.64527700	0.85354300
C	-0.67706700	3.52672700	2.08743800
C	-5.19149800	1.71374800	1.82449500
C	-8.58386600	1.42025800	0.03479100
C	-7.84654100	-3.37987700	0.00075500
C	-4.33058000	-2.17453200	1.61210900
C	0.31501900	-3.51782900	2.07534500
C	-4.91790100	-3.43143600	-1.31485300
C	5.57218500	-2.41649600	-1.71462500
H	0.96789700	-3.02944500	-1.96109300
H	3.05362300	-1.90662800	-2.49569200
H	5.12736800	-0.66911500	-3.71602700
H	4.76731600	1.74963000	-3.64241900
H	5.07074800	3.79055000	-2.50976600
H	5.46342100	3.85248100	-0.81565900
H	2.40183300	2.24683300	-2.10971200
H	0.12014600	2.96797400	-1.69256300
H	-0.91147300	6.14311500	-1.24210100
H	-0.86902500	5.74348800	0.44814300
H	-2.19094300	4.89286300	-2.80713600
H	-4.31369000	3.70755400	-3.07674900
H	-6.24356800	2.82784000	-2.15105100
H	-6.43510000	2.64031800	-0.42926700
H	-4.01482600	0.92949000	-2.65934500
H	-3.61423600	-1.49038500	-2.65311600
H	-3.20580300	-4.48166800	-3.10097800
H	-0.91333300	-5.27306100	-2.78547400
H	0.55690400	-5.67301300	0.51378600
H	0.54493700	-6.22489500	-1.13384000
H	1.93040200	-7.63783800	0.33524500
H	3.25482000	-7.90638000	1.48746300
H	1.99550500	-6.71591200	1.86261700
H	6.95788900	-4.97827000	-1.41681600
H	7.23284900	-4.26632100	0.19559800
H	7.18845300	-6.02299200	0.00804700
H	6.77593700	-2.31333700	1.17928200
H	5.72147300	-1.86505100	2.52735000

H	5.02049400	-2.64925700	1.09448700
H	3.85453500	3.17332300	1.19244700
H	4.70716100	2.63081500	2.65703100
H	5.57877400	3.57415700	1.43903100
H	5.65493100	6.14432800	-1.31107800
H	5.59068000	7.33280800	0.01168900
H	5.91805900	5.63401400	0.37919900
H	1.30911200	8.54705900	1.21412400
H	0.08083100	7.91900000	0.09608700
H	0.31398600	7.16184300	1.69567300
H	-0.43054600	4.56839600	2.30271400
H	-0.62967000	2.95650700	3.01420300
H	0.04213700	3.11816700	1.37514000
H	-5.40432700	0.86595600	1.17468800
H	-4.98210000	1.35300300	2.83110200
H	-6.06272700	2.37296400	1.86573000
H	-8.66555300	1.92659100	-0.92862100
H	-9.57580600	1.12472600	0.37590200
H	-8.15646900	2.10280100	0.77289700
H	-8.88304100	-3.40094400	0.33641300
H	-7.76610700	-3.87921300	-0.96607500
H	-7.23695800	-3.90841200	0.73778900
H	-5.23114300	-2.78022700	1.50514900
H	-4.22886300	-1.87660900	2.65521100
H	-4.41637300	-1.28391600	0.98690800
H	0.62256800	-4.50572100	2.42783300
H	1.02828200	-3.14894200	1.33662900
H	0.29734900	-2.83501300	2.92381300
H	-5.24001100	-3.97995600	-2.20578100
H	-5.44836400	-3.88715500	-0.48032800
H	5.91810500	-2.63196100	-2.73055200
H	6.38420000	-2.70995600	-1.05419600
H	2.93639500	-0.29895200	0.80430000
H	2.58549100	-0.08590100	-1.14191800

Total energy: -3970.4281521 a.u.

BSSE corrected energy: -3970.4599270 a.u.

4. Guest 6@benzo[6]juril 1

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	-1.88562400	0.72305500	3.41970000
C	0.46231900	0.44117300	2.75361900
C	0.98594700	-0.06686500	0.39907500
C	2.78069400	0.08428000	2.02815600
C	1.84144500	0.39797000	3.07050800
C	2.37860300	-0.12522700	0.75523800
C	-2.28745400	0.47249100	2.15728900
C	0.03567200	0.19829500	1.41604800
C	-1.34495300	0.22775700	1.10311900
C	-0.48995900	0.72353200	3.76436000
C	-0.04190100	0.97197900	5.06235900
C	-1.75042800	0.02059700	-0.21454200
C	2.24963700	0.65277600	4.38208200
C	1.31294400	0.93923600	5.36481700
C	0.53852800	-0.26375900	-0.91027600
C	-0.81531000	-0.21820000	-1.21150200
H	-2.62052000	0.91613700	4.19336300
H	3.82681800	0.01594700	2.30190300
H	3.09834100	-0.36281000	-0.01969700
H	-3.34213100	0.43343500	1.91594900
H	-0.76858600	1.18374500	5.83953800
H	-2.80629500	0.05836900	-0.45275800
H	3.30863100	0.62862400	4.61770800
H	1.64138900	1.13397800	6.37951000
H	1.26596700	-0.43993800	-1.69417600
H	-1.14454500	-0.36497600	-2.23448300
C	4.33430700	-4.43095400	-0.63638500
C	2.96311500	-4.23882500	-0.79505200
C	2.58400800	-3.10316400	-1.50560600
C	3.51395200	-2.19888900	-1.99649100
C	4.88711900	-2.36855600	-1.82768000
C	5.27765300	-3.53464800	-1.17394500
N	5.05369800	-5.44211700	-0.00207800
C	6.41103200	-5.22369100	-0.15228000
N	6.53996700	-4.04019800	-0.86241200
O	7.31194100	-5.93074100	0.24568000
C	5.37300600	0.75087500	-0.85898900
C	4.79807900	2.02380700	-0.68111500
C	5.33817200	0.10189000	-2.09062900
C	4.72517000	0.79780600	-3.13426000

C	4.19100700	2.06673200	-2.96516100
C	4.22297300	2.72326100	-1.73531200
N	5.88586000	0.37199500	0.37776700
C	5.63839600	1.36051600	1.31556400
N	4.97058000	2.37120600	0.65361600
O	5.92389000	1.32407600	2.49595400
C	3.72835000	4.14170000	-1.61809100
C	1.74113400	5.59375400	-0.99039700
C	2.27217100	4.32679400	-1.23401400
C	1.37221200	3.26586400	-1.18585100
C	0.00594700	3.45890500	-0.99343900
C	-0.54101900	4.72957900	-0.83780900
C	0.36688100	5.78847300	-0.79001500
N	2.34093400	6.85226900	-0.94062900
C	1.38537000	7.81876900	-0.67950300
N	0.16997000	7.15909800	-0.61899500
O	1.57767300	9.00631700	-0.51995800
C	-2.03509700	4.98957900	-0.81963100
C	-3.67345300	3.17497800	-0.07341200
C	-2.94423400	3.81186600	-1.06822800
C	-3.19156600	3.39184300	-2.37595600
C	-4.15259700	2.43855500	-2.66981000
C	-4.94347100	1.84290300	-1.68276900
C	-4.67580700	2.22904600	-0.37195600
N	-3.65948200	3.34098100	1.30678400
C	-4.62513800	2.53989300	1.88422500
N	-5.24654000	1.86375600	0.84418500
O	-4.86393300	2.41986400	3.06774900
C	-5.99762800	0.83245900	-2.08226200
C	-6.32598000	-1.62946500	-1.40429300
C	-5.53870800	-0.60945000	-1.93185100
C	-4.24090400	-0.97046400	-2.29475200
C	-3.72387600	-2.23176800	-2.04635300
C	-4.46952000	-3.22370500	-1.41296100
C	-5.79500800	-2.90606600	-1.13233700
N	-7.65614800	-1.64482800	-0.98458500
C	-7.97474600	-2.89604500	-0.48009500
N	-6.81596100	-3.64949800	-0.54196700
O	-9.06069400	-3.26250700	-0.08576900
C	-1.67563600	-3.97446100	0.22149200
C	-2.33549800	-4.53911800	-0.86797500
C	-1.53454700	-5.20244500	-1.79932500
C	-0.17020300	-5.36599400	-1.61589400
C	0.48912300	-4.86862500	-0.49147300

C	-0.28393000	-4.12807500	0.39737000
N	-2.14418100	-3.27584900	1.32805600
C	-1.09211100	-2.99039200	2.18673000
N	0.04614100	-3.50177900	1.59041200
O	-1.15674100	-2.41545600	3.25059000
C	1.93864400	-5.22270600	-0.26168900
C	4.58143200	-6.57347100	0.76743700
C	7.83428900	-3.65599400	-1.38313600
C	6.61305700	-0.81948500	0.75314100
C	4.31728100	3.42704100	1.40171300
C	3.74213100	7.21180100	-0.94733700
C	-1.01318300	7.87322900	-0.18792200
C	-2.63318500	3.95894600	2.12255600
C	-6.31398500	0.92929700	1.11774500
C	-8.71371700	-0.69845500	-1.26916900
C	-6.84317500	-5.04563700	-0.16073500
C	-3.46315300	-2.74960800	1.60330000
C	1.35004700	-3.25887000	2.16978200
C	-3.83738700	-4.54857500	-1.03492000
C	5.85249400	-1.30091400	-2.32100200
H	1.52812100	-2.91321500	-1.65654500
H	3.16443700	-1.31055800	-2.50931700
H	4.67697600	0.32747900	-4.11081700
H	3.74841800	2.57592900	-3.81464500
H	3.88047800	4.62068400	-2.59112700
H	4.37200500	4.68215200	-0.92505200
H	1.73966800	2.25772900	-1.33424400
H	-0.65049500	2.59579400	-1.00571600
H	-2.24936000	5.71681700	-1.60886000
H	-2.32352800	5.48078200	0.10898900
H	-2.63689900	3.85712500	-3.18394300
H	-4.32703500	2.16565300	-3.70545600
H	-6.26579800	1.02110400	-3.12659500
H	-6.90320200	1.00316900	-1.50599900
H	-3.59505600	-0.21562400	-2.72861000
H	-2.68683600	-2.43558000	-2.28577200
H	-2.00845000	-5.64330100	-2.66991700
H	0.40051700	-5.93326200	-2.34366700
H	2.10460500	-5.38438500	0.80401000
H	2.10920700	-6.19261200	-0.73762200
H	3.94826700	-7.22692900	0.16668700
H	5.46728300	-7.12571600	1.07904500
H	4.03600500	-6.24812600	1.65566100
H	7.78126700	-3.49292900	-2.46114100

H	8.22298800	-2.75977400	-0.89504300
H	8.51517300	-4.48035100	-1.17270600
H	7.58644800	-0.86003900	0.25793100
H	6.77402300	-0.75903400	1.82880600
H	6.04050300	-1.71866700	0.52595900
H	3.26410100	3.48991800	1.12366000
H	4.39890700	3.16626600	2.45617700
H	4.80288300	4.39310600	1.24551800
H	4.22877800	6.90899300	-1.87477900
H	3.78256500	8.29704200	-0.86022200
H	4.26743300	6.77268900	-0.09510700
H	-0.71352300	8.91073600	-0.04457900
H	-1.80433200	7.83419700	-0.93703200
H	-1.38608600	7.47751300	0.75974000
H	-2.77544000	5.03930500	2.20412500
H	-2.70867300	3.52223300	3.11717200
H	-1.64653600	3.73991500	1.70955200
H	-6.11476300	-0.03808000	0.65594700
H	-6.35875300	0.80994100	2.19972700
H	-7.27709000	1.31397600	0.77251900
H	-8.65535600	-0.35987500	-2.30514400
H	-9.65678200	-1.22046900	-1.10924300
H	-8.68272200	0.16353600	-0.59930000
H	-7.88819000	-5.30058500	0.01286000
H	-6.44522600	-5.67390600	-0.95840600
H	-6.28555700	-5.22443100	0.76155900
H	-4.20735200	-3.54441400	1.68202400
H	-3.39269500	-2.23290500	2.55998300
H	-3.76692000	-2.04058100	0.83113400
H	1.74111400	-4.14741000	2.67310700
H	2.04907600	-2.92474300	1.40267000
H	1.22924000	-2.46708100	2.90897000
H	-4.08143200	-5.29586300	-1.79672400
H	-4.28283400	-4.91599500	-0.11023700
H	6.02113100	-1.43198300	-3.39451900
H	6.82380500	-1.41994900	-1.84836400

Total energy: -4046.6454001 a.u.

BSSE corrected energy: -4046.6786181 a.u.

5. Guest 7@benzo[6]juril 1

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	1.09181000	0.99535100	3.62974200
C	1.98631400	-0.11321500	1.59379800
C	0.37503000	-0.68700500	-0.23229700
C	3.08745100	-0.60413000	0.87461700
C	-0.18609100	1.08017500	3.04332100
C	0.63971700	-0.10079300	1.01754000
C	-0.43478300	0.43584300	1.75163200
C	2.18145600	0.31744400	2.91935100
C	3.44031300	0.12032500	3.51169500
C	-1.73342300	0.34248000	1.22226700
C	4.31930400	-0.76403800	1.46825700
C	4.49154200	-0.42874200	2.81048300
C	-0.90315400	-0.74802800	-0.74333500
C	-1.97100100	-0.23372800	-0.00578800
H	3.60349500	0.39666900	4.54457800
H	-2.57106000	0.71100500	1.79849700
H	5.14455200	-1.16384000	0.88860300
H	5.45412100	-0.55463600	3.29000400
H	-1.07366800	-1.21110400	-1.70782800
H	-2.98250100	-0.29789300	-0.39097600
C	4.99629000	-3.22400700	-1.53430100
C	3.63526100	-3.45567600	-1.71222200
C	2.92598000	-2.42854300	-2.33760600
C	3.51552700	-1.22316200	-2.68126000
C	4.87243400	-0.96193300	-2.46572600
C	5.60950000	-2.02540400	-1.95804100
N	6.00661300	-4.02031000	-0.99562400
C	7.23267000	-3.39789000	-1.14549400
N	6.98019300	-2.15460600	-1.71323200
O	8.31844800	-3.85509400	-0.86486800
C	4.84028700	1.85864000	-0.64268600
C	3.87981300	2.60169500	0.07213900
C	4.62715600	1.47956000	-1.96721200
C	3.48873300	2.01510000	-2.57109100
C	2.54770400	2.75273900	-1.86958400
C	2.68366600	3.01404500	-0.50695300
N	5.88436800	1.61210000	0.23970900
C	5.61363300	2.17809900	1.47274400
N	4.36617600	2.75840100	1.36555100
O	6.33676400	2.16924600	2.44831400

C	1.55742100	3.61509700	0.31556300
C	-0.15831000	5.18841300	-0.79455300
C	0.30464100	3.92118900	-0.46449300
C	-0.48395300	2.85287000	-0.89196000
C	-1.69428500	3.03436600	-1.53138300
C	-2.22624200	4.30501700	-1.76123500
C	-1.40791000	5.37593100	-1.42144800
N	0.38203800	6.45361000	-0.58342600
C	-0.47841900	7.42327200	-1.06604300
N	-1.59306800	6.75173500	-1.54365300
O	-0.28864400	8.62092400	-1.08831600
C	-3.66003600	4.46635000	-2.24041800
C	-4.71103200	2.62482800	-0.79231200
C	-4.49015600	3.22109700	-2.03621300
C	-4.99948700	2.54453500	-3.14025300
C	-5.67965900	1.33944200	-3.02275500
C	-5.87106600	0.71455800	-1.79382800
C	-5.35866200	1.37927500	-0.67853100
N	-4.34100700	3.00594200	0.49493300
C	-4.70508900	2.02895300	1.39376100
N	-5.34174000	1.03834100	0.67241900
O	-4.49349900	2.02917400	2.59384900
C	-6.60021300	-0.60748400	-1.73162300
C	-6.05952400	-2.88057400	-0.67731400
C	-5.69876000	-1.80396700	-1.48277100
C	-4.42161100	-1.85709900	-2.03967900
C	-3.53536600	-2.88722000	-1.75702500
C	-3.85508100	-3.92153700	-0.88159300
C	-5.14687400	-3.90371500	-0.35803000
N	-7.23982200	-3.15936100	0.01047100
C	-7.09693300	-4.33353900	0.73208600
N	-5.80115200	-4.76851300	0.51811600
O	-7.94718300	-4.87919900	1.40197500
C	-0.55521800	-4.15189400	0.14552600
C	-1.39558400	-4.73133400	-0.80125300
C	-0.78004000	-5.20454200	-1.96132200
C	0.59611200	-5.16511800	-2.13318000
C	1.45476200	-4.68031200	-1.14411700
C	0.84684000	-4.17146200	0.00069300
N	-0.82750400	-3.57239100	1.37598000
C	0.35615500	-3.25820900	2.02367500
N	1.38142800	-3.62838200	1.16277700
O	0.47208800	-2.76828400	3.12419100
C	2.95089500	-4.76077600	-1.33982300

C	5.93192700	-5.34039000	-0.40808200
C	8.06131200	-1.47494600	-2.40433100
C	7.12947100	0.92398200	0.01897800
C	3.80385800	3.48581000	2.48284300
C	1.70934600	6.80366200	-0.12921300
C	-2.62378600	7.47008500	-2.26002700
C	-3.65696400	4.19167700	0.97687300
C	-5.73381400	-0.18910200	1.33294300
C	-8.55377900	-2.57032800	-0.13897000
C	-5.34321400	-5.99512800	1.13502000
C	-2.10127600	-3.17692400	1.93722500
C	2.73608900	-3.72966600	1.66215300
C	-2.85903100	-5.01475300	-0.55045600
C	5.42963800	0.43633100	-2.72112300
H	1.86787800	-2.57295400	-2.52438800
H	2.88946900	-0.43830600	-3.08701200
H	3.31124400	1.80627600	-3.62109100
H	1.65904500	3.09337400	-2.38465300
H	1.90053700	4.49311100	0.85778500
H	1.28308300	2.88128000	1.08198600
H	-0.13749600	1.84684300	-0.69549100
H	-2.27299200	2.15844300	-1.79467700
H	-3.68430400	4.71483100	-3.30547200
H	-4.12191500	5.31255100	-1.72719700
H	-4.84417700	2.96994400	-4.12567800
H	-6.06435000	0.85844000	-3.91569500
H	-7.12928200	-0.74312300	-2.68019600
H	-7.37172100	-0.55165100	-0.96711700
H	-4.09916400	-1.04429100	-2.68117300
H	-2.54752500	-2.87697000	-2.20095100
H	-1.39831400	-5.65766800	-2.72938900
H	1.02846100	-5.56376700	-3.04485700
H	3.40159300	-5.17601100	-0.44072900
H	3.14459700	-5.49152500	-2.13213400
H	5.47675400	-6.05393100	-1.09654000
H	6.95739800	-5.64687400	-0.20508000
H	5.37603100	-5.32613200	0.53223800
H	7.79125100	-1.30273600	-3.44848300
H	8.32186900	-0.52603300	-1.93507600
H	8.93173600	-2.12870700	-2.35443000
H	7.70348700	1.39995700	-0.78062100
H	7.69393800	0.99515500	0.94825500
H	6.96335000	-0.13003500	-0.21330100
H	2.82368900	3.09724400	2.75696400

H	4.48795200	3.34102300	3.31811000
H	3.73468600	4.55476800	2.26500500
H	2.45993600	6.20024700	-0.64465600
H	1.85972900	7.85605100	-0.36772200
H	1.81303400	6.67395500	0.95111400
H	-2.26659300	8.49207100	-2.38449400
H	-2.79183400	7.02340200	-3.24155400
H	-3.56420900	7.49614400	-1.70506700
H	-4.01409900	5.07747600	0.45470300
H	-3.89081200	4.28385600	2.03657100
H	-2.57646900	4.10116600	0.85676700
H	-5.12687900	-1.02916400	0.99154000
H	-5.56747200	-0.03249700	2.39779900
H	-6.78869900	-0.41016500	1.17018100
H	-8.78369700	-2.40877600	-1.19326300
H	-9.26601100	-3.27813000	0.28448000
H	-8.64634400	-1.62682700	0.40479600
H	-6.21243200	-6.44242900	1.61586700
H	-4.95032500	-6.68739100	0.38971300
H	-4.58421000	-5.80276200	1.89688200
H	-2.62179200	-4.02303700	2.39506600
H	-1.89354900	-2.43623800	2.70897500
H	-2.72686200	-2.72677600	1.16674900
H	2.98191500	-4.76803400	1.91036100
H	3.44837400	-3.33669100	0.94030000
H	2.79009500	-3.12167000	2.56427500
H	-3.11919800	-5.90919700	-1.12637600
H	-2.96926200	-5.29886200	0.49512700
H	5.36398600	0.65813300	-3.79057100
H	6.48312000	0.48445300	-2.46363600
H	2.98089300	-0.87822500	-0.16474600
H	1.18191500	-1.12511200	-0.80211500
C	1.30518200	1.62570800	4.86858200
C	-1.19784300	1.79830300	3.70646600
C	-0.96333600	2.40379600	4.92161800
C	0.29862700	2.31431500	5.50962800
H	0.49322700	2.79174000	6.46331400
H	-1.76112000	2.95009900	5.41140100
H	-2.18436000	1.89586400	3.27015200
H	2.28160900	1.59024500	5.33337200

Total energy: -4124.0559427 a.u.

BSSE corrected energy: -4124.0875543 a.u.

6. Guest 8@benzo[6]juril 1

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	-0.00295200	1.72813100	4.12813900
C	1.23983500	0.75836400	2.18395700
C	-0.00080500	-0.13123100	0.25785400
C	2.40556100	-0.23297100	0.29536000
C	2.40676500	0.36249900	1.56644700
C	1.22847000	-0.46126800	-0.35776100
C	-1.24750700	1.41934600	3.50203900
C	-0.00150200	0.48809100	1.53725100
C	-1.24352300	0.75719600	2.18313800
C	1.24230900	1.41996400	3.50314000
C	-2.42180900	1.76854800	4.13871900
C	-2.41618300	2.40010900	5.39427600
C	-1.23486400	2.69496600	6.01426100
C	-0.00369300	2.37429400	5.39479900
C	2.41585700	1.76939600	4.14108500
C	1.22675500	2.69530700	6.01551900
C	2.40877700	2.40079300	5.39671700
C	-1.22936800	-0.46293400	-0.35829200
C	-2.40967200	0.35975000	1.56514200
C	-2.40706900	-0.23614200	0.29424800
H	3.34205700	-0.53206400	-0.15731500
H	3.35364600	0.48796600	2.07261800
H	1.21700200	-0.93004400	-1.33538600
H	-3.38338300	1.57733400	3.67781700
H	-3.36129200	2.65201100	5.86149400
H	-1.22146000	3.18371500	6.98277500
H	3.37796200	1.57859300	3.68112800
H	1.21222000	3.18401600	6.98403700
H	3.35335500	2.65288700	5.86490600
H	-1.21681800	-0.93186700	-1.33582200
H	-3.35695100	0.48429800	2.07080700
H	-3.34295000	-0.53670000	-0.15871900
C	5.13897900	-3.95767100	-0.86371600
C	3.75852200	-4.05112000	-1.02849800
C	3.16559800	-3.04552700	-1.78805200
C	3.88932800	-1.97160300	-2.28571800
C	5.26186400	-1.83756100	-2.07753700
C	5.87975100	-2.89016000	-1.40656900
N	6.04618800	-4.78265600	-0.20127100
C	7.32921700	-4.28619300	-0.34444600

N	7.21502300	-3.10962700	-1.06840500
O	8.35427000	-4.78811400	0.06391700
C	5.07846700	1.31534700	-1.06544200
C	4.28020000	2.46300300	-0.90203400
C	5.20224600	0.68557700	-2.30158700
C	4.50716000	1.27275800	-3.36085900
C	3.75706000	2.42841000	-3.20537600
C	3.63585500	3.06864700	-1.97264900
N	5.60832800	1.02269800	0.18852000
C	5.14292800	1.93225500	1.12203400
N	4.33592400	2.81935200	0.44096900
O	5.37808900	1.92405300	2.31597300
C	2.92924800	4.39578900	-1.87717700
C	0.69512900	5.55160200	-1.61229300
C	1.42942800	4.36641600	-1.65326800
C	0.69443300	3.18547700	-1.58244200
C	-0.70006600	3.18385400	-1.58420000
C	-1.43762400	4.36308800	-1.65683900
C	-0.70620600	5.54998600	-1.61409600
N	1.10175500	6.88617800	-1.63404400
C	-0.00797000	7.71399200	-1.60889000
N	-1.11575000	6.88366200	-1.63692900
O	-0.00943100	8.92601200	-1.55387800
C	-2.93694300	4.38894600	-1.88446400
C	-4.28487300	2.45514200	-0.90737700
C	-3.64102000	3.06037400	-1.97854600
C	-3.76071100	2.41830600	-3.21045400
C	-4.50890100	1.26123100	-3.36469500
C	-5.20349000	0.67436600	-2.30493500
C	-5.08130300	1.30606400	-1.06960300
N	-4.34172800	2.81319500	0.43513800
C	-5.14769800	1.92577700	1.11701700
N	-5.61118900	1.01421500	0.18452300
O	-5.38344600	1.91884000	2.31085000
C	-5.98924700	-0.59673100	-2.53769300
C	-5.87358400	-2.90104800	-1.40435800
C	-5.25803100	-1.84848800	-2.07752400
C	-3.88532600	-1.98028000	-2.28604600
C	-3.15935400	-3.05194500	-1.78681300
C	-3.74999000	-4.05731700	-1.02518100
C	-5.13052000	-3.96609200	-0.85977000
N	-7.20831700	-3.12254700	-1.06542800
C	-7.31995600	-4.29792500	-0.33913400
N	-6.03591100	-4.79163400	-0.19552700

O	-8.34388400	-4.80104300	0.07057300
C	-0.70056600	-4.26366900	0.46356400
C	-1.42966700	-5.01330900	-0.45688700
C	-0.68802900	-5.70170100	-1.41809500
C	0.69822200	-5.70070700	-1.41909800
C	1.44026800	-5.01133400	-0.45890400
C	0.71143100	-4.26279300	0.46265400
N	-1.10259500	-3.46991300	1.52845600
C	0.00574000	-2.97830300	2.20021200
N	1.11384800	-3.46869100	1.52714800
O	0.00591300	-2.27185200	3.18344000
C	2.94115000	-5.17703300	-0.42344100
C	5.82555800	-6.02417700	0.50931900
C	8.40747400	-2.47331900	-1.58703000
C	6.49823200	-0.04278200	0.59107200
C	3.46139900	3.72520000	1.16128800
C	2.41892300	7.45005000	-1.42869200
C	-2.43469700	7.44476200	-1.43545800
C	-3.46902800	3.72137600	1.15473000
C	-6.50059500	-0.05137600	0.58784200
C	-8.40216000	-2.48956400	-1.58491700
C	-5.81251600	-6.03085300	0.51819300
C	-2.43741600	-3.16365300	1.99295400
C	2.44887300	-3.16115800	1.99022700
C	-2.93026900	-5.18111400	-0.41933200
C	5.99052900	-0.58366400	-2.53584900
H	2.09610300	-3.08880400	-1.95507300
H	3.36319000	-1.18088000	-2.80874100
H	4.57844500	0.81439400	-4.34168500
H	3.26647000	2.86634200	-4.06815900
H	3.10617700	4.91738700	-2.82343300
H	3.41585300	5.00537500	-1.11642000
H	1.21896400	2.23638400	-1.56471500
H	-1.22247000	2.23357000	-1.56771000
H	-3.11259400	4.90818200	-2.83226700
H	-3.42661000	4.99921400	-1.12622800
H	-3.27052300	2.85590300	-4.07363600
H	-4.57900800	0.80144400	-4.34494000
H	-6.20151500	-0.67354600	-3.60868400
H	-6.95538400	-0.52216100	-2.04554600
H	-3.36089700	-1.18948300	-2.81067000
H	-2.08988400	-3.09355100	-1.95440600
H	-1.21901500	-6.28663100	-2.16166000
H	1.22895200	-6.28484400	-2.16346800

H	3.25331600	-5.33455900	0.60950500
H	3.17595800	-6.10766200	-0.94860300
H	5.26717000	-6.73191600	-0.10334600
H	6.81004300	-6.43728300	0.72594000
H	5.29988900	-5.85890300	1.45242100
H	8.32195300	-2.32154200	-2.66435800
H	8.60825700	-1.51815400	-1.09685200
H	9.23916900	-3.14563900	-1.37805000
H	7.47843800	0.06316200	0.12099700
H	6.61981600	0.04339500	1.66997600
H	6.07511400	-1.01912100	0.35412300
H	2.42494200	3.56971400	0.85566900
H	3.55829700	3.49487100	2.22097000
H	3.74455700	4.76835900	1.00672200
H	3.10273400	7.18255700	-2.23435400
H	2.29252600	8.53194900	-1.41349700
H	2.83782400	7.13046300	-0.47083500
H	-2.31059800	8.52693000	-1.42027600
H	-3.11565200	7.17554900	-2.24297300
H	-2.85561700	7.12463700	-0.47866600
H	-3.75279900	4.76394800	0.99741900
H	-3.56746000	3.49332000	2.21476300
H	-2.43196500	3.56611700	0.85109600
H	-6.07688200	-1.02770100	0.35195500
H	-6.62255000	0.03575700	1.66662400
H	-7.48071700	0.05363800	0.11736600
H	-8.31714200	-2.33941700	-2.66251600
H	-9.23243500	-3.16323700	-1.37465700
H	-8.60480900	-1.53400500	-1.09628500
H	-6.79610600	-6.44517900	0.73653000
H	-5.25324500	-6.73922200	-0.09292700
H	-5.28656800	-5.86210400	1.46052800
H	-2.89586500	-4.02649500	2.48471800
H	-2.34114100	-2.35609600	2.71762700
H	-3.06296200	-2.82762300	1.16609000
H	2.90908000	-4.02391900	2.48047700
H	3.07291900	-2.82343900	1.16290300
H	2.35240600	-2.35449700	2.71587700
H	-3.16434400	-6.11280900	-0.94293400
H	-3.24094400	-5.33771700	0.61419000
H	6.20321900	-0.65860400	-3.60689200
H	6.95638400	-0.50774600	-2.04337600

Total energy: -4200.2626947 a.u.

BSSE corrected energy: -4200.2963798 a.u.

7. Guest 3@benzo[6]juril 2

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	-1.00959900	-0.81181600	2.75691600
C	-0.75690000	-0.33483000	0.38146000
C	1.45541200	0.18455300	-0.56115700
C	-0.51298200	0.16813300	-1.97135300
C	-1.30772100	-0.16975200	-0.92226500
C	0.88783100	0.34613400	-1.78738000
C	0.40247300	-0.64081400	2.93765800
C	0.64887400	-0.15125300	0.56691700
C	1.19556900	-0.31209800	1.83792200
C	-1.55143000	-0.66163200	1.47800700
C	0.95826100	-0.82966900	4.24047600
C	-1.81740800	-1.14578900	3.88998200
C	0.16045500	-1.16077200	5.28957000
C	-1.24570300	-1.31478200	5.11229400
H	2.52423900	0.29497800	-0.41557100
H	-0.94388100	0.30361800	-2.95744600
H	-2.37290700	-0.32317000	-1.05440800
H	1.49749900	0.60884300	-2.64382300
H	2.26263600	-0.18267600	1.97530300
H	-2.60889200	-0.82545300	1.32394300
H	2.03001300	-0.73541000	4.35974800
H	-2.89049100	-1.23909200	3.75306700
H	0.59199100	-1.31140800	6.27228700
H	-1.86327500	-1.56803300	5.96670300
C	-2.52567700	5.64490400	-0.54292100
C	-1.31867600	4.95824900	-0.67723400
C	-1.41864700	3.60919300	-0.99529700
C	-2.64828500	2.98297000	-1.14958200
C	-3.85732400	3.64642000	-0.97842700
C	-3.76287500	5.00255300	-0.67145200
N	-2.79420600	6.99517200	-0.26913900
C	-4.16469100	7.21039600	-0.28409300
N	-4.75194300	5.97268100	-0.46343700
O	-4.73274900	8.27837300	-0.17167100
C	-5.01352700	0.49673500	-0.38136100
C	-5.05158100	-0.88388900	-0.64826600
C	-5.09325100	1.45538300	-1.38646100
C	-5.12336300	0.96677300	-2.68919100
C	-5.11433800	-0.39437700	-2.96152200
C	-5.10001600	-1.36391000	-1.95868400

N	-4.94837500	0.65087700	1.00814800
C	-4.99203200	-0.58988400	1.60817200
N	-5.06078500	-1.52761100	0.59795000
O	-4.94179600	-0.82621000	2.80325800
C	-5.12760500	-2.82737700	-2.33875000
C	-3.70311400	-4.79304900	-1.51723200
C	-3.80629100	-3.53103700	-2.08289700
C	-2.59679900	-2.88244500	-2.32870000
C	-1.37182600	-3.43556900	-1.98885300
C	-1.27126400	-4.66963200	-1.34884200
C	-2.47502200	-5.31778300	-1.09372100
N	-4.68865100	-5.71053000	-1.13494500
C	-4.11623900	-6.73552300	-0.39673800
N	-2.74818800	-6.51279300	-0.40705300
O	-4.71396700	-7.64972500	0.12714700
C	0.06298500	-5.29548900	-0.99418500
C	2.03160800	-3.80954500	-0.26465900
C	1.29411900	-4.46146100	-1.25027700
C	1.81186100	-4.40101200	-2.54417100
C	3.01818700	-3.78382500	-2.83028000
C	3.80835400	-3.19886800	-1.84064200
C	3.27886900	-3.21009800	-0.55023800
N	1.81198700	-3.64973000	1.11033700
C	2.89423900	-3.01000100	1.68359400
N	3.79354300	-2.75766800	0.66667400
O	3.05114000	-2.73172800	2.85644300
C	5.18199000	-2.67426500	-2.20689900
C	6.46092300	-0.54703400	-1.55251000
C	5.34064400	-1.17100300	-2.08405700
C	4.28734300	-0.32967500	-2.43271400
C	4.30297700	1.02542100	-2.14724600
C	5.35486100	1.63056700	-1.46096100
C	6.45130000	0.81590000	-1.20871200
N	7.66076200	-1.08594700	-1.06852100
C	8.39022300	-0.09593400	-0.44829300
N	7.65187800	1.06791500	-0.53233100
O	9.50570200	-0.22002100	0.02943700
C	3.04261100	3.39074400	0.25625800
C	3.85137400	3.59904000	-0.86137800
C	3.29045200	4.36691000	-1.88114400
C	2.03931600	4.95311900	-1.76873200
C	1.25246400	4.80597000	-0.62920400
C	1.75968300	3.96535100	0.35815400
N	3.26923100	2.70652300	1.45848100

C	2.19510200	2.88771500	2.29671700
N	1.25763700	3.63009500	1.62187500
O	2.08518700	2.45853400	3.44102200
C	0.01271900	5.64874000	-0.47581900
C	-1.89275800	8.12381200	-0.24755200
C	-6.19088000	5.84666000	-0.52235800
C	-4.63333400	1.83182600	1.78869800
C	-4.97433900	-2.92993300	0.96395700
C	-6.06189600	-5.81519800	-1.55438700
C	-1.92861200	-7.10893000	0.62853900
C	0.70479100	-4.06482600	1.95632600
C	5.03790500	-2.09390200	1.00611000
C	8.40298600	-2.27928300	-1.48792300
C	8.18370000	2.30468700	-0.02000700
C	4.50726900	2.15601500	2.00875900
C	-0.08485500	3.71073100	2.18932000
C	5.26292000	3.08259200	-1.02286800
C	-5.18760700	2.93285900	-1.11280300
O	-6.96143100	-5.11561900	-0.73051100
O	-1.79063600	-6.29454500	1.75523100
O	-0.54674900	-3.77139800	1.41511800
O	4.95310000	-0.70850700	0.98156500
O	9.55841900	-1.96288300	-2.19034700
O	7.60892200	2.69882500	1.19980300
O	4.24885700	1.05907300	2.83676700
O	-0.83581000	2.55668700	1.98529200
O	-1.30359600	8.38775000	-1.49246200
O	-6.67846000	5.66438500	-1.82395800
O	-5.74133400	2.66225400	2.01671300
O	-3.66085500	-3.36798200	1.16509200
H	-0.51714700	3.01777500	-1.10700200
H	-2.66224400	1.93114000	-1.39306700
H	-5.17291200	1.67674900	-3.50753300
H	-5.14548600	-0.72583900	-3.99402300
H	-5.38473700	-2.89283600	-3.40072900
H	-5.94065100	-3.31864000	-1.80241600
H	-2.61846000	-1.89736400	-2.77862100
H	-0.46781100	-2.87577600	-2.19664400
H	0.16956300	-6.21633500	-1.57912000
H	0.05686500	-5.60962600	0.04580500
H	1.25958800	-4.88474200	-3.34287500
H	3.38699900	-3.79024400	-3.85048000
H	5.39783700	-2.98850000	-3.23309200
H	5.91675800	-3.18526500	-1.58275200

H	3.39844400	-0.76947600	-2.87043900
H	3.43750900	1.62793500	-2.39447700
H	3.87708000	4.54160500	-2.77676300
H	1.67672700	5.58973700	-2.56816200
H	0.03907000	6.10617600	0.51960900
H	0.08210700	6.48258800	-1.17991400
H	-1.07434100	7.93767200	0.44319200
H	-2.49004600	8.96353300	0.11450900
H	-6.50365800	4.98162500	0.05642800
H	-6.58191900	6.75629800	-0.06133500
H	-3.88877300	2.42471800	1.26162200
H	-4.20512900	1.46225000	2.72272900
H	-5.41393800	-3.53356600	0.17937500
H	-5.56992300	-3.04006200	1.87252000
H	-6.29862100	-6.88129500	-1.57350800
H	-6.16390200	-5.39654600	-2.55433200
H	-2.44430200	-8.01591800	0.94044900
H	-0.96291300	-7.38026300	0.19452900
H	0.87879100	-3.57329900	2.91664000
H	0.71582000	-5.14745000	2.10129900
H	5.80335400	-2.39636000	0.29866900
H	5.30535800	-2.46035600	1.99990400
H	7.77335900	-2.85570400	-2.15798000
H	8.62163800	-2.86596300	-0.58884400
H	9.26079200	2.15162100	0.07404900
H	7.98616200	3.10742100	-0.72806800
H	5.03176400	2.94464500	2.56058900
H	5.13605700	1.80308800	1.19812700
H	0.05337400	3.92090100	3.25253600
H	-0.62310200	4.52491300	1.71809500
H	5.75919900	3.71455500	-1.76683500
H	5.81496500	3.23068300	-0.09343700
H	-5.76444100	3.40731300	-1.91191700
H	-5.76340300	3.07324700	-0.19620700
H	-7.00393400	-5.57864000	0.10946500
H	-1.58659600	-5.38485500	1.49308000
H	-0.69935300	-2.82102500	1.36575300
H	4.59992800	-0.37759500	1.82190800
H	10.14534400	-1.51850200	-1.56849100
H	7.86249000	2.06052500	1.87027900
H	3.54346700	1.32600900	3.45105700
H	-0.48165900	1.85537800	2.54140200
H	-1.98574300	8.70628500	-2.08661300
H	-6.56266100	6.48719000	-2.30266600

H	-6.34298900	2.20230300	2.60517800
H	-3.38344700	-3.12554900	2.05150700

Total energy: -4719.4346682 a.u.

BSSE corrected energy: -4719.5020388 a.u.

8. Guest 4@benzo[6]juril 2

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	-1.00959900	-0.81181600	2.75691600
C	-0.75690000	-0.33483000	0.38146000
C	1.45541200	0.18455300	-0.56115700
C	-0.51298200	0.16813300	-1.97135300
C	-1.30772100	-0.16975200	-0.92226500
C	0.88783100	0.34613400	-1.78738000
C	0.40247300	-0.64081400	2.93765800
C	0.64887400	-0.15125300	0.56691700
C	1.19556900	-0.31209800	1.83792200
C	-1.55143000	-0.66163200	1.47800700
C	0.95826100	-0.82966900	4.24047600
C	-1.81740800	-1.14578900	3.88998200
C	0.16045500	-1.16077200	5.28957000
C	-1.24570300	-1.31478200	5.11229400
H	2.52423900	0.29497800	-0.41557100
H	-0.94388100	0.30361800	-2.95744600
H	-2.37290700	-0.32317000	-1.05440800
H	1.49749900	0.60884300	-2.64382300
H	2.26263600	-0.18267600	1.97530300
H	-2.60889200	-0.82545300	1.32394300
H	2.03001300	-0.73541000	4.35974800
H	-2.89049100	-1.23909200	3.75306700
H	0.59199100	-1.31140800	6.27228700
H	-1.86327500	-1.56803300	5.96670300
C	-2.52567700	5.64490400	-0.54292100
C	-1.31867600	4.95824900	-0.67723400
C	-1.41864700	3.60919300	-0.99529700
C	-2.64828500	2.98297000	-1.14958200
C	-3.85732400	3.64642000	-0.97842700
C	-3.76287500	5.00255300	-0.67145200
N	-2.79420600	6.99517200	-0.26913900
C	-4.16469100	7.21039600	-0.28409300
N	-4.75194300	5.97268100	-0.46343700
O	-4.73274900	8.27837300	-0.17167100
C	-5.01352700	0.49673500	-0.38136100
C	-5.05158100	-0.88388900	-0.64826600
C	-5.09325100	1.45538300	-1.38646100
C	-5.12336300	0.96677300	-2.68919100
C	-5.11433800	-0.39437700	-2.96152200
C	-5.10001600	-1.36391000	-1.95868400

N	-4.94837500	0.65087700	1.00814800
C	-4.99203200	-0.58988400	1.60817200
N	-5.06078500	-1.52761100	0.59795000
O	-4.94179600	-0.82621000	2.80325800
C	-5.12760500	-2.82737700	-2.33875000
C	-3.70311400	-4.79304900	-1.51723200
C	-3.80629100	-3.53103700	-2.08289700
C	-2.59679900	-2.88244500	-2.32870000
C	-1.37182600	-3.43556900	-1.98885300
C	-1.27126400	-4.66963200	-1.34884200
C	-2.47502200	-5.31778300	-1.09372100
N	-4.68865100	-5.71053000	-1.13494500
C	-4.11623900	-6.73552300	-0.39673800
N	-2.74818800	-6.51279300	-0.40705300
O	-4.71396700	-7.64972500	0.12714700
C	0.06298500	-5.29548900	-0.99418500
C	2.03160800	-3.80954500	-0.26465900
C	1.29411900	-4.46146100	-1.25027700
C	1.81186100	-4.40101200	-2.54417100
C	3.01818700	-3.78382500	-2.83028000
C	3.80835400	-3.19886800	-1.84064200
C	3.27886900	-3.21009800	-0.55023800
N	1.81198700	-3.64973000	1.11033700
C	2.89423900	-3.01000100	1.68359400
N	3.79354300	-2.75766800	0.66667400
O	3.05114000	-2.73172800	2.85644300
C	5.18199000	-2.67426500	-2.20689900
C	6.46092300	-0.54703400	-1.55251000
C	5.34064400	-1.17100300	-2.08405700
C	4.28734300	-0.32967500	-2.43271400
C	4.30297700	1.02542100	-2.14724600
C	5.35486100	1.63056700	-1.46096100
C	6.45130000	0.81590000	-1.20871200
N	7.66076200	-1.08594700	-1.06852100
C	8.39022300	-0.09593400	-0.44829300
N	7.65187800	1.06791500	-0.53233100
O	9.50570200	-0.22002100	0.02943700
C	3.04261100	3.39074400	0.25625800
C	3.85137400	3.59904000	-0.86137800
C	3.29045200	4.36691000	-1.88114400
C	2.03931600	4.95311900	-1.76873200
C	1.25246400	4.80597000	-0.62920400
C	1.75968300	3.96535100	0.35815400
N	3.26923100	2.70652300	1.45848100

C	2.19510200	2.88771500	2.29671700
N	1.25763700	3.63009500	1.62187500
O	2.08518700	2.45853400	3.44102200
C	0.01271900	5.64874000	-0.47581900
C	-1.89275800	8.12381200	-0.24755200
C	-6.19088000	5.84666000	-0.52235800
C	-4.63333400	1.83182600	1.78869800
C	-4.97433900	-2.92993300	0.96395700
C	-6.06189600	-5.81519800	-1.55438700
C	-1.92861200	-7.10893000	0.62853900
C	0.70479100	-4.06482600	1.95632600
C	5.03790500	-2.09390200	1.00611000
C	8.40298600	-2.27928300	-1.48792300
C	8.18370000	2.30468700	-0.02000700
C	4.50726900	2.15601500	2.00875900
C	-0.08485500	3.71073100	2.18932000
C	5.26292000	3.08259200	-1.02286800
C	-5.18760700	2.93285900	-1.11280300
O	-6.96143100	-5.11561900	-0.73051100
O	-1.79063600	-6.29454500	1.75523100
O	-0.54674900	-3.77139800	1.41511800
O	4.95310000	-0.70850700	0.98156500
O	9.55841900	-1.96288300	-2.19034700
O	7.60892200	2.69882500	1.19980300
O	4.24885700	1.05907300	2.83676700
O	-0.83581000	2.55668700	1.98529200
O	-1.30359600	8.38775000	-1.49246200
O	-6.67846000	5.66438500	-1.82395800
O	-5.74133400	2.66225400	2.01671300
O	-3.66085500	-3.36798200	1.16509200
H	-0.51714700	3.01777500	-1.10700200
H	-2.66224400	1.93114000	-1.39306700
H	-5.17291200	1.67674900	-3.50753300
H	-5.14548600	-0.72583900	-3.99402300
H	-5.38473700	-2.89283600	-3.40072900
H	-5.94065100	-3.31864000	-1.80241600
H	-2.61846000	-1.89736400	-2.77862100
H	-0.46781100	-2.87577600	-2.19664400
H	0.16956300	-6.21633500	-1.57912000
H	0.05686500	-5.60962600	0.04580500
H	1.25958800	-4.88474200	-3.34287500
H	3.38699900	-3.79024400	-3.85048000
H	5.39783700	-2.98850000	-3.23309200
H	5.91675800	-3.18526500	-1.58275200

H	3.39844400	-0.76947600	-2.87043900
H	3.43750900	1.62793500	-2.39447700
H	3.87708000	4.54160500	-2.77676300
H	1.67672700	5.58973700	-2.56816200
H	0.03907000	6.10617600	0.51960900
H	0.08210700	6.48258800	-1.17991400
H	-1.07434100	7.93767200	0.44319200
H	-2.49004600	8.96353300	0.11450900
H	-6.50365800	4.98162500	0.05642800
H	-6.58191900	6.75629800	-0.06133500
H	-3.88877300	2.42471800	1.26162200
H	-4.20512900	1.46225000	2.72272900
H	-5.41393800	-3.53356600	0.17937500
H	-5.56992300	-3.04006200	1.87252000
H	-6.29862100	-6.88129500	-1.57350800
H	-6.16390200	-5.39654600	-2.55433200
H	-2.44430200	-8.01591800	0.94044900
H	-0.96291300	-7.38026300	0.19452900
H	0.87879100	-3.57329900	2.91664000
H	0.71582000	-5.14745000	2.10129900
H	5.80335400	-2.39636000	0.29866900
H	5.30535800	-2.46035600	1.99990400
H	7.77335900	-2.85570400	-2.15798000
H	8.62163800	-2.86596300	-0.58884400
H	9.26079200	2.15162100	0.07404900
H	7.98616200	3.10742100	-0.72806800
H	5.03176400	2.94464500	2.56058900
H	5.13605700	1.80308800	1.19812700
H	0.05337400	3.92090100	3.25253600
H	-0.62310200	4.52491300	1.71809500
H	5.75919900	3.71455500	-1.76683500
H	5.81496500	3.23068300	-0.09343700
H	-5.76444100	3.40731300	-1.91191700
H	-5.76340300	3.07324700	-0.19620700
H	-7.00393400	-5.57864000	0.10946500
H	-1.58659600	-5.38485500	1.49308000
H	-0.69935300	-2.82102500	1.36575300
H	4.59992800	-0.37759500	1.82190800
H	10.14534400	-1.51850200	-1.56849100
H	7.86249000	2.06052500	1.87027900
H	3.54346700	1.32600900	3.45105700
H	-0.48165900	1.85537800	2.54140200
H	-1.98574300	8.70628500	-2.08661300
H	-6.56266100	6.48719000	-2.30266600

H	-6.34298900	2.20230300	2.60517800
H	-3.38344700	-3.12554900	2.05150700

Total energy: -4873.0885669 a.u.

BSSE corrected energy: -4873.1530255 a.u.

9. Guest 5@benzo[6]juril 2

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	-1.80062600	-0.06085000	1.44237300
C	0.63900700	0.13364600	1.29739900
C	1.61712000	0.39170000	-1.00027800
C	1.87054600	0.23609100	1.96875900
C	-1.93304400	0.07745100	0.10868000
C	0.50994100	0.23764800	-0.14643600
C	-0.78069500	0.25512600	-0.72428500
C	-0.52355200	-0.01674400	2.07706800
C	-0.43399700	-0.07228100	3.48368900
C	-0.91978900	0.47731300	-2.10765100
C	1.94662700	0.19791900	3.34332300
C	0.78156100	0.04418900	4.11193300
C	1.45870600	0.61589900	-2.34709200
C	0.17814500	0.66883400	-2.90975900
H	-2.66547000	-0.18605300	2.07146000
H	-2.91814200	0.06372000	-0.33980200
H	-1.34874700	-0.18425300	4.05561400
H	-1.91578900	0.52050600	-2.52632700
H	2.90953200	0.25026100	3.83896000
H	0.84794100	0.01211100	5.19347900
H	2.33497400	0.76435400	-2.96813000
H	0.05467700	0.85962400	-3.96955400
C	3.70043200	-4.83249600	-1.03395500
C	2.40163500	-4.38145600	-1.25605500
C	2.28138900	-3.06716100	-1.69752500
C	3.38680500	-2.24070800	-1.82253500
C	4.67537100	-2.65225700	-1.50957600
C	4.81548400	-3.99527800	-1.18224800
N	4.18146900	-6.07667400	-0.59023200
C	5.56201100	-6.03395500	-0.52839500
N	5.94728400	-4.74467000	-0.82653600
O	6.31508300	-6.96966700	-0.31234600
C	5.22595900	0.14380300	0.28806800
C	4.98645100	1.48995500	0.63893200
C	5.38811200	-0.24940700	-1.03741000
C	5.20002000	0.74735000	-1.99565900
C	4.89922300	2.05580400	-1.65105800
C	4.80121000	2.48003600	-0.32410700
N	5.33118700	-0.58685000	1.47971500
C	5.17176200	0.27270000	2.55627100

N	4.98499800	1.54141600	2.03830500
O	5.17041100	-0.03814900	3.73126900
C	4.51823900	3.94544100	-0.06559200
C	2.65136500	5.64259100	-0.51620400
C	3.06167300	4.34248100	-0.23335500
C	2.03771700	3.41693900	-0.08508000
C	0.69745300	3.73635200	-0.24129500
C	0.27982300	5.03196900	-0.52473100
C	1.29640000	5.97863300	-0.65691800
N	3.38620400	6.82088300	-0.71827100
C	2.53311700	7.86278700	-1.02797800
N	1.24870400	7.35404900	-0.94282500
O	2.84797000	9.00087800	-1.31753400
C	-1.18247500	5.41209700	-0.64598800
C	-2.77685800	3.55536500	0.20250000
C	-2.21139700	4.31607400	-0.82080300
C	-2.77777700	4.14784500	-2.08363900
C	-3.89129600	3.35214100	-2.29671500
C	-4.52630100	2.66466100	-1.26249800
C	-3.92317300	2.75524400	-0.00772500
N	-2.46036500	3.45990600	1.56045100
C	-3.33142100	2.59145600	2.18058100
N	-4.26335100	2.20376900	1.23561600
O	-3.27972900	2.23283000	3.34369000
C	-5.81709700	1.92777000	-1.55996600
C	-6.49690700	-0.50760900	-1.08621100
C	-5.65442500	0.42376100	-1.67297200
C	-4.54193400	-0.09673100	-2.33087900
C	-4.19200700	-1.43334200	-2.25214100
C	-4.94866100	-2.34719700	-1.51839500
C	-6.14692900	-1.86882100	-1.00012500
N	-7.67614000	-0.33692900	-0.35241200
C	-8.06155000	-1.55025600	0.16045700
N	-7.11207700	-2.48526600	-0.18975300
O	-9.11624500	-1.78621700	0.73846100
C	-2.18594600	-3.71219600	-0.09013400
C	-2.94684300	-3.92040000	-1.23983500
C	-2.25444300	-4.39790900	-2.35149100
C	-0.91238700	-4.74564800	-2.29565700
C	-0.16442100	-4.62919900	-1.12634300
C	-0.81532100	-4.03858100	-0.04492000
N	-2.54573800	-3.30819000	1.20160300
C	-1.45803900	-3.42024800	2.03007200
N	-0.38959400	-3.80728600	1.26589800

O	-1.43568700	-3.21412700	3.24445400
C	1.19760100	-5.27469200	-1.04424600
C	3.50714200	-7.35728400	-0.56897100
C	7.35415800	-4.55851800	-1.19020300
C	5.07900900	-2.01035700	1.69603600
C	4.70614400	2.65755800	2.92666500
C	4.81008300	7.03941200	-0.65800800
C	0.12005700	8.20495300	-1.23099600
C	-1.34786900	3.98430300	2.34543000
C	-5.32872400	1.29859300	1.62902100
C	-8.70981000	0.69892900	-0.45368900
C	-7.53285900	-3.88513900	-0.09639800
C	-3.87276600	-3.01169600	1.74983600
C	0.92569000	-3.94297300	1.89598300
C	-4.44907900	-3.76307600	-1.30574200
C	5.80668900	-1.64112700	-1.45770600
H	1.29766800	-2.65942700	-1.90274500
H	3.23273100	-1.21563000	-2.11805000
H	5.31535700	0.48811900	-3.04309000
H	4.75821600	2.79394700	-2.43328400
H	5.12613100	4.51090200	-0.77521700
H	4.84256400	4.23805000	0.93287600
H	2.29828100	2.40163300	0.16388600
H	-0.03937500	2.95223000	-0.11760100
H	-1.29255100	6.07494200	-1.50669600
H	-1.47117700	6.01581900	0.22360700
H	-2.36054600	4.70746800	-2.91338000
H	-4.32003300	3.29859700	-3.29198800
H	-6.22242800	2.32808800	-2.49476100
H	-6.54738800	2.17971300	-0.79349300
H	-3.89119000	0.59276400	-2.85417200
H	-3.26356000	-1.76353000	-2.70405300
H	-2.80434500	-4.56254700	-3.27192500
H	-0.44131800	-5.18460800	-3.16818000
H	1.27664400	-5.76657700	-0.07106700
H	1.23545500	-6.08625300	-1.77672600
H	2.63353200	-7.31667200	0.07662000
H	4.23364100	-8.05794700	-0.15089500
H	7.47981800	-3.55519900	-1.58237400
H	7.94525300	-4.67432400	-0.27599300
H	5.33042200	-2.18124900	2.74469900
H	5.74324300	-2.59783900	1.06673100
H	5.46126300	3.43309800	2.78825100
H	4.80328100	2.24131600	3.93272200

H	5.21929100	6.53808200	0.21677600
H	4.94023400	8.11903400	-0.55614900
H	-0.66535700	8.03942800	-0.49718300
H	0.49468800	9.22683800	-1.14028200
H	-1.78331900	4.37020600	3.27165500
H	-0.87696200	4.79274200	1.79747700
H	-6.22779400	1.55432000	1.07374100
H	-5.49675800	1.49503400	2.68957100
H	-8.33502800	1.49168500	-1.09296300
H	-8.88728600	1.08878200	0.55503600
H	-6.75281200	-4.51440200	-0.50922900
H	-7.66289300	-4.10809600	0.96713100
H	-4.32876400	-3.95179000	2.08785200
H	-4.47709700	-2.56188900	0.96613200
H	0.89580800	-4.81867400	2.55515000
H	1.67264500	-4.07772400	1.11958700
H	-4.82022100	-4.40589500	-2.11072600
H	-4.87065300	-4.17329400	-0.38739500
H	6.29122700	-1.56614100	-2.43710900
H	6.58010500	-1.98137500	-0.76666600
H	2.77729600	0.33069900	1.39048700
H	2.62056800	0.34847400	-0.59832500
O	-0.45631900	7.96751700	-2.48802300
H	0.17452800	8.23322700	-3.15980700
O	5.50337900	6.53152700	-1.76687400
H	5.25754200	7.05086900	-2.53468200
O	-5.06414500	-0.04936300	1.39498000
H	-4.63686900	-0.46152700	2.15725800
O	-0.35937900	3.04129400	2.60334500
H	-0.72550500	2.37138800	3.18951200
O	-9.87715000	0.22963100	-1.03937100
H	-10.23641300	-0.43375200	-0.43954800
O	-8.68868900	-4.14549200	-0.82290300
H	-9.40362500	-3.68024100	-0.37692100
O	3.04364300	-7.75315300	-1.83011800
H	3.80249900	-7.92750600	-2.39045000
O	7.76629200	-5.43845400	-2.18490800
H	7.74423700	-6.31839500	-1.79305100
O	3.78129000	-2.39648100	1.38147700
H	3.15236200	-2.17847700	2.08214100
O	3.47608600	3.26347000	2.69585900
H	2.75704400	2.64530000	2.86434800
O	1.29620900	-2.80043500	2.59409000
H	0.63559200	-2.61973100	3.27392900

O	-3.82142900	-2.08967600	2.79435300
H	-3.10439900	-2.36224600	3.39013600

Total energy: -4873.0755871 a.u.

BSSE corrected energy: -4873.1410730 a.u.

10. Guest 6@benzo[6]juril 2

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	-2.17742000	1.97657600	3.53955500
C	0.20907400	1.85252800	2.98765600
C	0.89826200	0.73414900	0.90568900
C	2.58445200	1.64598800	2.40090400
C	1.56567000	2.10715000	3.30594800
C	2.26214000	1.01390400	1.24975400
C	-2.48303900	1.30193600	2.40926600
C	-0.12400000	1.15634800	1.78595800
C	-1.47551000	0.86286000	1.48463700
C	-0.81105100	2.27573000	3.87707400
C	1.87588000	2.78785600	4.48452800
C	-1.78406900	0.14696700	0.32557700
C	0.55850100	0.01145200	-0.23719700
C	0.86997700	3.21528900	5.33954400
C	-0.76846700	-0.27750000	-0.52097100
C	-0.46085500	2.96191800	5.04209700
H	-2.96904400	2.30030400	4.20672000
H	3.62170400	1.78176500	2.69182600
H	3.02479800	0.64976200	0.57315300
H	-3.51638300	1.08013900	2.19515100
H	2.91634200	2.97980000	4.72433900
H	-2.81752000	-0.09982300	0.10628100
H	1.35113700	-0.33330800	-0.89273000
H	1.12614900	3.74699700	6.24849700
H	-1.01576100	-0.84413000	-1.41119600
H	-1.24275600	3.29056700	5.71826400
C	4.24348100	-4.78569800	-0.44125700
C	2.87485100	-4.54077400	-0.39608300
C	2.43676500	-3.40053900	-1.06526000
C	3.32066300	-2.52202100	-1.67408100
C	4.69428400	-2.73842900	-1.67995800
C	5.12779500	-3.92897200	-1.10902800
N	5.01773000	-5.80816600	0.12728200
C	6.33862800	-5.63699700	-0.23882600
N	6.41915300	-4.45376800	-0.94334900
O	7.26037700	-6.40897900	-0.03383800
C	5.21179200	0.48208800	-0.94075400
C	4.90529400	1.85559500	-0.93752200
C	5.15913300	-0.27150600	-2.11025800
C	4.68648900	0.38366900	-3.24536400

C	4.30663200	1.71637300	-3.21856400
C	4.40892900	2.49922000	-2.06895300
N	5.62216800	0.14194400	0.35736500
C	5.59129200	1.27510700	1.15494900
N	5.18355500	2.32510800	0.35179500
O	5.84676100	1.32768500	2.34203800
C	3.94227700	3.93163300	-2.11602300
C	1.91851100	5.38351200	-1.56671900
C	2.46318200	4.12522800	-1.81861100
C	1.55327500	3.06992300	-1.83028300
C	0.18154900	3.26270100	-1.70135700
C	-0.37221500	4.52920400	-1.54102400
C	0.54011400	5.57383200	-1.40095600
N	2.51762000	6.64278800	-1.42979200
C	1.55305900	7.59691300	-1.12641300
N	0.32964400	6.93636700	-1.15597800
O	1.74097400	8.76833800	-0.89895500
C	-1.86127200	4.80590200	-1.63530500
C	-3.62764300	3.11631000	-0.83664000
C	-2.75922400	3.60750200	-1.80575800
C	-2.78931500	2.95809400	-3.04042300
C	-3.65873000	1.91444600	-3.30338500
C	-4.54894800	1.42907600	-2.34465600
C	-4.48375400	2.02475400	-1.08822800
N	-3.88967800	3.54080800	0.47189900
C	-4.85572900	2.73590000	1.04419400
N	-5.21904800	1.80310000	0.08566200
O	-5.29158400	2.81303500	2.17583300
C	-5.54116400	0.35673000	-2.72891500
C	-6.07699000	-1.93144600	-1.72863800
C	-5.16186000	-1.03036600	-2.25104600
C	-3.82708600	-1.42396300	-2.20983800
C	-3.42688100	-2.60539200	-1.60675900
C	-4.32844500	-3.45562300	-0.96674500
C	-5.66534300	-3.08258800	-1.04205700
N	-7.46510100	-1.82614300	-1.56738500
C	-7.91571700	-2.86724100	-0.78696200
N	-6.81528000	-3.64408400	-0.47125200
O	-9.07551800	-3.08080300	-0.47818800
C	-1.63379700	-4.06105100	0.81775700
C	-2.37674900	-4.82677800	-0.08060600
C	-1.65718100	-5.73595100	-0.85198000
C	-0.28875600	-5.90399700	-0.71416700
C	0.46232300	-5.15461400	0.18692900

C	-0.23552200	-4.19794100	0.92175000
N	-2.01539000	-3.07679700	1.73812300
C	-0.90162100	-2.64467400	2.42044300
N	0.19101200	-3.27761300	1.88520500
O	-0.88975600	-1.85100400	3.35850300
C	1.92762600	-5.46279400	0.34275600
C	4.59871200	-7.04333900	0.75145800
C	7.63013300	-4.27103600	-1.74974000
C	5.60137400	-1.15827500	1.02120500
C	5.12440500	3.66524200	0.89426000
C	3.91196200	6.99901400	-1.45039000
C	-0.80971700	7.54025300	-0.48892900
C	-3.27428800	4.59548500	1.25069500
C	-6.02369800	0.66123900	0.49360100
C	-8.46345800	-1.13753200	-2.39217100
C	-6.92573000	-4.70405000	0.49745700
C	-3.33334900	-2.80292600	2.31540300
C	1.51391000	-3.03444100	2.46933300
C	-3.86760300	-4.72163400	-0.26842800
C	5.65291000	-1.69239800	-2.20899100
O	4.61546900	6.58503500	-0.30505200
O	-0.95734500	7.14100500	0.83933000
O	-1.88270200	4.47821000	1.32987800
O	-5.29130200	-0.50561300	0.70299600
O	-9.26665000	-2.02368600	-3.09712700
O	-6.34223200	-4.37755900	1.73452300
O	-3.51085000	-1.44845800	2.59088200
O	1.80509900	-1.67976300	2.56971100
O	3.94792900	-7.91503200	-0.13113400
O	7.87652200	-5.35264400	-2.58736600
O	4.32368300	-1.69174200	1.17102700
O	3.83543900	4.21399400	0.89292600
H	1.37704000	-3.17404300	-1.07663900
H	2.93719400	-1.61208000	-2.12084100
H	4.62852200	-0.16767100	-4.17780800
H	3.92271000	2.17812700	-4.12179800
H	4.13644000	4.30710400	-3.12652600
H	4.53638300	4.55182900	-1.44958900
H	1.92117800	2.06113900	-1.97211100
H	-0.47384000	2.40178300	-1.75236600
H	-2.01416700	5.45493200	-2.50577400
H	-2.18495100	5.38811900	-0.78068500
H	-2.12292300	3.30795200	-3.82146500
H	-3.67438800	1.47234500	-4.29399200

H	-5.64635400	0.36652900	-3.81869800
H	-6.51814500	0.63650400	-2.33378300
H	-3.07530500	-0.75563100	-2.61438000
H	-2.37385400	-2.85944700	-1.59478500
H	-2.19625000	-6.34497700	-1.56920800
H	0.21939900	-6.65268400	-1.31157900
H	2.18171300	-5.47508200	1.40785700
H	2.09246400	-6.48441300	-0.00915500
H	3.89367800	-6.83539200	1.55220800
H	5.50750400	-7.48025200	1.17077100
H	7.49788600	-3.40092500	-2.38261700
H	8.45817400	-4.09905400	-1.05489900
H	6.10240800	-0.99145600	1.97677900
H	6.17058600	-1.87609900	0.43653100
H	5.73828200	4.34581800	0.30408200
H	5.53900700	3.58151900	1.90109900
H	3.94250600	8.08731500	-1.51412200
H	4.37669700	6.57060600	-2.34315500
H	-0.61273800	8.61076800	-0.48116000
H	-1.70709600	7.34801300	-1.08233900
H	-3.75820900	4.54801100	2.22812600
H	-3.47216400	5.57012500	0.80209200
H	-6.75337400	0.43206900	-0.27912300
H	-6.54537000	0.99496300	1.39292900
H	-7.93925300	-0.53330700	-3.12588900
H	-9.05425300	-0.49092700	-1.73360800
H	-7.99393700	-4.91181200	0.58876400
H	-6.41044800	-5.59449000	0.14331200
H	-3.43710800	-3.39972700	3.22977800
H	-4.10410000	-3.08885100	1.60878200
H	1.54489200	-3.52226100	3.45130400
H	2.26783900	-3.45726600	1.81335800
H	-4.18554100	-5.58425200	-0.86257100
H	-4.37076900	-4.82335300	0.69565500
H	5.89056500	-1.89599900	-3.25849000
H	6.60003300	-1.75646300	-1.66774700
H	4.05751400	5.99035300	0.21235400
H	-1.07792100	6.18396500	0.90860200
H	-1.65128600	3.73006000	1.88800400
H	-4.79416600	-0.50274900	1.53301200
H	-9.78592700	-2.50654000	-2.44474400
H	-6.83235100	-3.64623100	2.11690100
H	-2.77454700	-1.16272500	3.15197200
H	1.12922600	-1.26827800	3.12347100

H	4.58871800	-8.23274700	-0.77043300
H	8.10617800	-6.09243000	-2.01474400
H	3.81374300	-1.23440100	1.85050600
H	3.21971000	3.62237700	1.33838500

Total energy: -4949.3079167 a.u.

BSSE corrected energy: -4949.3717066 a.u.

11. Guest 7@benzo[6]juril 2

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	1.35184600	1.53509100	3.62071200
C	2.11322700	0.22770400	1.64527400
C	0.43534600	-0.22756000	-0.15379700
C	3.11102600	-0.53372700	1.01247200
C	0.01098400	1.37282500	3.22614400
C	0.74733800	0.26500700	1.12328700
C	-0.29471700	0.72248500	1.94961600
C	2.41072700	0.85401500	2.87057400
C	3.70937200	0.72183500	3.39642200
C	-1.61539300	0.56144900	1.50936200
C	4.35925500	-0.69366700	1.57253300
C	4.66923900	-0.04135400	2.76641000
C	-0.87162600	-0.35220300	-0.57574800
C	-1.90947900	0.01767600	0.27938100
H	3.95700200	1.18288900	4.34312400
H	-2.43353200	0.84595400	2.15453100
H	5.09046000	-1.32521700	1.08374800
H	5.65612700	-0.13965400	3.20143400
H	-1.08689900	-0.74192700	-1.56513300
H	-2.94317200	-0.12614500	-0.00313500
C	4.01689200	-4.23120300	-0.47908200
C	2.64523900	-4.01526500	-0.39776500
C	2.12218100	-3.11377400	-1.32361200
C	2.92894400	-2.43089300	-2.21741900
C	4.30846700	-2.63479200	-2.30112000
C	4.82377800	-3.61691600	-1.46043700
N	4.85792600	-5.05364900	0.27744300
C	6.12426100	-5.04660300	-0.27258300
N	6.10952800	-4.15258900	-1.31724700
O	7.06605500	-5.74617100	0.06114500
C	5.38335800	0.37942900	-1.79165200
C	4.92634600	1.65748400	-1.40468600
C	4.86093700	-0.27781900	-2.90273900
C	3.95214200	0.45137000	-3.67168000
C	3.56167000	1.73496600	-3.33271100
C	4.01649300	2.37129500	-2.17644300
N	6.35175900	0.00857300	-0.85562600
C	6.47711400	0.99013900	0.10491700
N	5.59444800	1.99162700	-0.21994100
O	7.25005200	0.94355800	1.04966500

C	3.59022200	3.78885200	-1.90243900
C	1.64795500	5.29082800	-1.30773200
C	2.12521700	4.01157100	-1.58802300
C	1.16479400	3.00587700	-1.61696900
C	-0.19623900	3.27484500	-1.50386100
C	-0.68510400	4.56665800	-1.32760900
C	0.28208400	5.55743100	-1.15690600
N	2.32087000	6.51455300	-1.15273600
C	1.40578600	7.51920200	-0.87166200
N	0.15743500	6.92705400	-0.88652400
O	1.65446200	8.68690500	-0.64741100
C	-2.16067400	4.90341000	-1.41519000
C	-3.66633200	3.08563200	-0.47106300
C	-3.10190200	3.73898600	-1.55947400
C	-3.52793800	3.30655300	-2.81363900
C	-4.48343500	2.30996200	-2.96393000
C	-5.08994300	1.68610900	-1.87377300
C	-4.65311600	2.10105100	-0.61765400
N	-3.46097900	3.26471900	0.90028700
C	-4.30450400	2.43287200	1.60925800
N	-5.02983700	1.71435000	0.67552700
O	-4.37796200	2.33477500	2.82190000
C	-6.14654500	0.63051100	-2.08319900
C	-6.48525100	-1.81847700	-1.37549400
C	-5.65979800	-0.77993300	-1.80489600
C	-4.31195000	-1.10246500	-1.94841000
C	-3.79840100	-2.33966700	-1.58954600
C	-4.60412700	-3.35456900	-1.08353800
C	-5.96807800	-3.08154100	-1.04535200
N	-7.86845300	-1.87905600	-1.15765100
C	-8.23086600	-3.16061000	-0.78562800
N	-7.04984700	-3.88059000	-0.65045800
O	-9.35616100	-3.58366100	-0.62077900
C	-1.99808200	-3.83884500	0.80613500
C	-2.53764800	-4.57708700	-0.24493700
C	-1.62957300	-5.30564900	-1.01110200
C	-0.27545100	-5.32752300	-0.72370600
C	0.27710900	-4.60408700	0.33388000
C	-0.61188600	-3.82979000	1.07655200
N	-2.59748200	-3.05076900	1.79006400
C	-1.63896500	-2.59171300	2.65984100
N	-0.42069400	-3.00794700	2.19355500
O	-1.87797100	-1.94121900	3.67677200
C	1.75872600	-4.75362200	0.58948100

C	4.54838500	-5.95842500	1.36034700
C	7.24630800	-4.22077900	-2.23701200
C	7.35108100	-1.04503200	-0.84162100
C	5.31873300	3.06915800	0.72606200
C	3.73508300	6.80199400	-1.10889000
C	-1.01135500	7.69224600	-0.50483400
C	-2.43157400	4.02745700	1.57160500
C	-6.06512800	0.79684500	1.09164200
C	-8.88303500	-0.86381000	-1.37045200
C	-7.10324800	-5.32144700	-0.50903300
C	-3.98832400	-2.74970400	2.11769000
C	0.82991900	-2.74568800	2.92939400
C	-4.00967500	-4.64803400	-0.56266000
C	5.10401200	-1.73482100	-3.23734600
H	1.05618900	-2.92407500	-1.32118500
H	2.47691700	-1.68829500	-2.86572900
H	3.53897200	-0.01108600	-4.56206300
H	2.86919400	2.26834400	-3.97484200
H	3.82004500	4.36044300	-2.81006600
H	4.18117400	4.23110200	-1.10725000
H	1.47891500	1.98105700	-1.76711900
H	-0.89905900	2.45294300	-1.58307100
H	-2.29873400	5.57044100	-2.27063600
H	-2.47549200	5.48522100	-0.55047600
H	-3.11200400	3.78473600	-3.69385700
H	-4.79101400	2.01546100	-3.96170300
H	-6.51836700	0.68863900	-3.10934500
H	-6.99618700	0.86821800	-1.44716200
H	-3.63182700	-0.33497600	-2.29961700
H	-2.73057900	-2.50809700	-1.65848800
H	-2.00742800	-5.89243000	-1.84100300
H	0.38755200	-5.93452700	-1.33073700
H	2.00829300	-4.45642800	1.60671600
H	1.99640600	-5.82000400	0.53105800
H	3.88499900	-5.46742300	2.06773100
H	5.50347500	-6.17239800	1.84444100
H	7.02490100	-3.61380200	-3.10910700
H	8.11633400	-3.81886400	-1.70659500
H	8.33500400	-0.57327600	-0.94275100
H	7.18356800	-1.69712800	-1.68836600
H	5.59526200	4.03154700	0.29703600
H	5.96498500	2.85378600	1.58163700
H	3.80208000	7.89110700	-1.05438300
H	4.22737000	6.45021600	-2.01385500

H	-1.60935500	7.11660600	0.19880700
H	-0.62199100	8.58484000	-0.00999400
H	-1.49572100	3.93149900	1.02425600
H	-2.31763500	3.58421500	2.56060400
H	-5.90656300	0.63012000	2.15678200
H	-5.95263100	-0.14853500	0.57057800
H	-8.64323400	0.02357500	-0.78891600
H	-9.80722200	-1.30564400	-0.99084200
H	-6.45513200	-5.65202600	0.29901700
H	-8.14161500	-5.54253800	-0.25086500
H	-4.21263300	-3.23241600	3.07535500
H	-4.63006400	-3.15012600	1.34300500
H	1.05897000	-3.64250100	3.52596800
H	1.61837100	-2.58261500	2.19277900
H	-4.18694400	-5.44793400	-1.28668200
H	-4.54221100	-4.95467600	0.34139100
H	4.77423100	-1.90857300	-4.26528600
H	6.16499100	-1.96497300	-3.22971600
H	2.89759400	-1.05418600	0.08921000
H	1.23318700	-0.51874000	-0.82387500
C	1.63275900	2.29045500	4.77089000
C	-1.00340000	1.88071300	4.05682900
C	-0.70568700	2.58731100	5.20238200
C	0.62561000	2.81781000	5.54911200
H	0.86999200	3.39735300	6.43197600
H	-1.50874900	2.96884600	5.82249800
H	-2.04639700	1.73002100	3.80892400
H	2.65958800	2.47360200	5.05927800
O	4.40069600	6.17702700	-0.04266900
H	3.93818000	6.37883500	0.77337600
O	-1.83978600	8.01697000	-1.58797700
H	-1.37173900	8.65059400	-2.13465700
O	-2.71880600	5.40102500	1.65758000
H	-3.45322000	5.51867900	2.26264600
O	-7.36010700	1.27127700	0.81062000
H	-7.53587500	2.03179800	1.36735800
O	-8.98556100	-0.47145900	-2.71036900
H	-9.35903600	-1.20105100	-3.20760800
O	-6.67193000	-6.00004900	-1.65543300
H	-7.31460500	-5.85559100	-2.35238700
O	-4.22882900	-1.38083100	2.18324400
H	-3.69928000	-1.04301700	2.91543500
O	0.76548700	-1.61069200	3.70826200
H	-0.10924700	-1.56472900	4.12225200

O	3.89781600	-7.12640400	0.94201100
H	4.52415300	-7.65562000	0.44402300
O	7.47586600	-5.51062300	-2.69853400
H	7.75644000	-6.02423000	-1.93267000
O	7.29355700	-1.82281400	0.31271800
H	7.53802900	-1.23367600	1.03650600
O	3.97292200	3.15992100	1.06115200
H	3.71622600	2.38411800	1.57076100

Total energy: -5026.7004102 a.u.

BSSE corrected energy: -5026.7688307 a.u.

12. Guest 8@benzo[6]juril 2

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	0.52285200	1.66187300	4.09673000
C	1.61302600	0.55541300	2.14782000
C	0.29725300	-0.02880200	0.15988400
C	2.68631000	-0.33940600	0.16304000
C	2.74086600	0.15219800	1.47448000
C	1.48449500	-0.46082600	-0.47549500
C	-0.68714600	1.78194300	3.35370600
C	0.36824500	0.53892800	1.46072800
C	-0.80379700	1.09169100	2.05353300
C	1.66159600	1.00628300	3.54760300
C	-1.71712200	2.53586800	3.87434300
C	0.60550500	2.22872100	5.39590500
C	-1.61975500	3.12522400	5.14721300
C	-0.49475900	2.95824500	5.90551800
C	2.78742000	0.85192100	4.32836500
C	1.79255100	2.06663300	6.15069200
C	2.85140700	1.37589300	5.63186100
C	-0.96128500	-0.15067200	-0.47117600
C	-2.00707400	0.95713300	1.39222300
C	-2.08650000	0.31223000	0.14619300
H	3.60777700	-0.63645000	-0.31851600
H	3.70135500	0.20649000	1.96057400
H	1.42536000	-0.87518200	-1.47541000
H	-2.61367000	2.71054700	3.29461100
H	-2.45281700	3.70904300	5.52261600
H	-0.42025900	3.39524200	6.89594700
H	3.63831800	0.30212600	3.95047600
H	1.84368300	2.49710700	7.14536800
H	3.75477000	1.23629700	6.21458800
H	-1.01925800	-0.62690400	-1.44460600
H	-2.91316200	1.34364100	1.83939000
H	-3.04734700	0.17249000	-0.32814300
C	5.66784600	-2.80804500	-1.17043300
C	4.36239400	-3.27915400	-1.26874200
C	3.53301700	-2.59350300	-2.15626900
C	3.93540100	-1.43123000	-2.79170900
C	5.21055300	-0.89268200	-2.61768200
C	6.09511800	-1.66645800	-1.87744600
N	6.75418100	-3.22728500	-0.39141100
C	7.84426200	-2.43816400	-0.67832200

N	7.44338200	-1.46317500	-1.55905900
O	8.98991000	-2.63505000	-0.29264400
C	4.31470000	2.06907600	-1.50715800
C	3.30738500	3.02027200	-1.23140000
C	4.46627800	1.51985600	-2.77948100
C	3.57670000	1.97700200	-3.75324800
C	2.63875200	2.96352400	-3.49658700
C	2.49732400	3.54117800	-2.23550900
N	5.03050300	1.90440800	-0.31627800
C	4.46383700	2.67966500	0.67677200
N	3.41053100	3.35320900	0.11814900
O	4.84671100	2.73510800	1.83705100
C	1.61482100	4.75487400	-2.07248700
C	-0.75366200	5.57413700	-1.66179700
C	0.13430700	4.51555800	-1.84994800
C	-0.44474100	3.25307600	-1.93745200
C	-1.82349900	3.07352800	-1.94995800
C	-2.71921300	4.13778000	-1.87115200
C	-2.14266500	5.39242800	-1.67927200
N	-0.52283300	6.94579500	-1.47273900
C	-1.72956900	7.60575800	-1.30739100
N	-2.72091700	6.65888400	-1.50769000
O	-1.88922500	8.77721200	-1.03329900
C	-4.21326400	3.95251300	-2.09072100
C	-5.01877100	1.77887700	-0.97613000
C	-4.66558300	2.51532800	-2.10452400
C	-4.70154000	1.83288500	-3.31861800
C	-5.08052600	0.50345500	-3.40895700
C	-5.43966300	-0.24066900	-2.28725200
C	-5.38103200	0.41924500	-1.06191100
N	-5.10034400	2.13618200	0.37138000
C	-5.53924200	1.06137500	1.10618000
N	-5.67339000	-0.00764200	0.24051700
O	-5.76244100	1.04496200	2.30934600
C	-5.90342400	-1.66491500	-2.45490100
C	-5.25638200	-3.89741300	-1.42628400
C	-4.88661200	-2.70590900	-2.03400800
C	-3.51865500	-2.47038100	-2.14060600
C	-2.57748100	-3.35075800	-1.62583000
C	-2.94456200	-4.50277600	-0.93488200
C	-4.31099200	-4.73857000	-0.82945100
N	-6.52462100	-4.40194500	-1.10209300
C	-6.38249400	-5.51820000	-0.30752200
N	-5.02569800	-5.73323400	-0.14567100

O	-7.29094800	-6.20448200	0.12916400
C	0.12487500	-4.21858400	0.51952900
C	-0.48303700	-5.04853900	-0.41925700
C	0.35472500	-5.59358400	-1.39035600
C	1.72254900	-5.37652900	-1.39191500
C	2.35467800	-4.60746400	-0.41564100
C	1.52245500	-4.02470800	0.54057300
N	-0.38934400	-3.52583800	1.61453600
C	0.64066700	-2.94888000	2.31911500
N	1.80963200	-3.24113500	1.66301400
O	0.49494100	-2.30283100	3.35411600
C	3.85763600	-4.46815800	-0.47182600
C	7.03747800	-4.48478600	0.29234900
C	8.49891500	-0.77838600	-2.31458800
C	6.22730900	1.15783700	0.01416600
C	2.56656300	4.20822900	0.96803000
C	0.71855600	7.62658700	-1.18549700
C	-4.10795200	7.01511800	-1.33686200
C	-4.96776500	3.45733400	1.00602300
C	-5.77378000	-1.34903000	0.81163300
C	-7.81682100	-4.23731300	-1.77648300
C	-4.55250300	-6.68270000	0.83138000
C	-1.74162100	-3.37256900	2.14710300
C	3.15114600	-2.98304400	2.21259100
C	-1.92759300	-5.47225000	-0.37045500
C	5.51038800	0.49163200	-3.16521600
O	1.33224800	7.18003800	-0.00613100
O	-4.67446400	6.49535700	-0.16268200
O	-4.46577500	3.36202800	2.29538800
O	-4.57243300	-2.03985400	0.86059300
O	-8.23174600	-5.40076000	-2.41119400
O	-4.00236500	-6.06675300	1.96795200
O	-2.13995900	-2.03798100	2.20077700
O	3.15153500	-2.18076200	3.33931000
O	7.80737200	-5.35086500	-0.47994400
O	9.42193700	-1.66058300	-2.85684300
O	5.98816800	0.00437700	0.76647300
O	2.16017900	3.57024200	2.12427300
H	2.51661700	-2.94160700	-2.29066700
H	3.21509300	-0.87875400	-3.38498300
H	3.65711900	1.57100400	-4.75604400
H	2.01564200	3.32927400	-4.30599500
H	1.70711400	5.32903100	-3.00153600
H	2.01676200	5.40078300	-1.29115400

H	0.19717800	2.38425100	-2.02675500
H	-2.21035300	2.06867300	-2.05097000
H	-4.45863300	4.38107300	-3.06864200
H	-4.78503700	4.53065000	-1.36503200
H	-4.42505900	2.36913900	-4.22006800
H	-5.11437800	0.02409400	-4.38124100
H	-6.18306400	-1.81072500	-3.50347600
H	-6.82272100	-1.79238800	-1.87984700
H	-3.18135100	-1.54834600	-2.60077200
H	-1.52325700	-3.12203000	-1.73060900
H	-0.08068300	-6.23902000	-2.14551100
H	2.33371200	-5.83920400	-2.15943800
H	4.25913000	-4.41876300	0.53747000
H	4.26471000	-5.38721000	-0.90738800
H	6.10614400	-4.99185000	0.51146800
H	7.53826200	-4.22303200	1.22832100
H	8.03740500	-0.25728100	-3.14774500
H	8.97380200	-0.05571600	-1.64048600
H	6.88457900	1.84148400	0.55782900
H	6.71415200	0.84679900	-0.90112400
H	1.66648900	4.45621800	0.41530500
H	3.12679600	5.12725700	1.17655000
H	0.46628700	8.68859600	-1.14839300
H	1.43719800	7.45185400	-1.98345800
H	-4.13568500	8.10650000	-1.36093400
H	-4.69902000	6.61796200	-2.15974000
H	-5.95042000	3.94637500	0.98860800
H	-4.26501800	4.05198000	0.43258100
H	-6.45218200	-1.94918700	0.20930200
H	-6.21358100	-1.19148000	1.79934600
H	-7.70769300	-3.47952000	-2.54537400
H	-8.54348700	-3.90239100	-1.02807100
H	-5.41463700	-7.30811700	1.07405600
H	-3.76279100	-7.30076200	0.40977400
H	-1.75314200	-3.82751800	3.14241800
H	-2.44595700	-3.88590000	1.50278300
H	3.59344400	-3.96049400	2.45407900
H	3.74047400	-2.50088500	1.42454200
H	-2.00523100	-6.41012800	-0.92992300
H	-2.18805600	-5.72099800	0.66138400
H	5.55496800	0.44981500	-4.25754300
H	6.49056300	0.84304100	-2.84726400
H	0.78434400	7.42638100	0.74187100
H	-4.27186500	6.92855100	0.59292000

H	-5.00743600	2.70700200	2.76164400
H	-3.93350600	-1.65542800	1.47822100
H	-8.39954400	-6.04861400	-1.71770300
H	-4.69244400	-5.56442600	2.40669200
H	-1.54374100	-1.56130100	2.79044400
H	2.23867300	-2.02677900	3.63754100
H	8.68781000	-4.96734100	-0.52938200
H	9.85805500	-2.09011900	-2.11152600
H	5.80943200	0.28383400	1.66778500
H	2.94606300	3.31884900	2.62392800

Total energy: -5102.8944816 a.u.

BSSE corrected energy: -5102.9612944 a.u.