

## Supporting Information for:

# Elucidating the Intercalation of Methylated 1,10-phenanthroline with DNA. The Important Weight of the CH/H Interactions and the Selectivity of CH/ $\pi$ and CH/n Interactions

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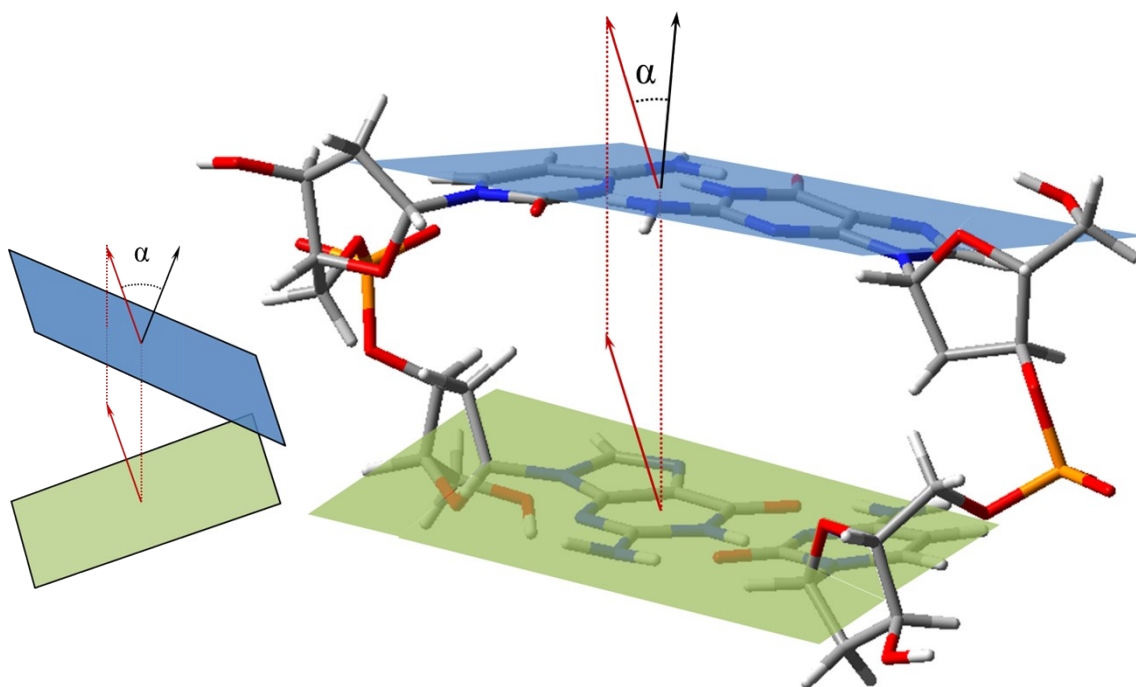
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## Geometries

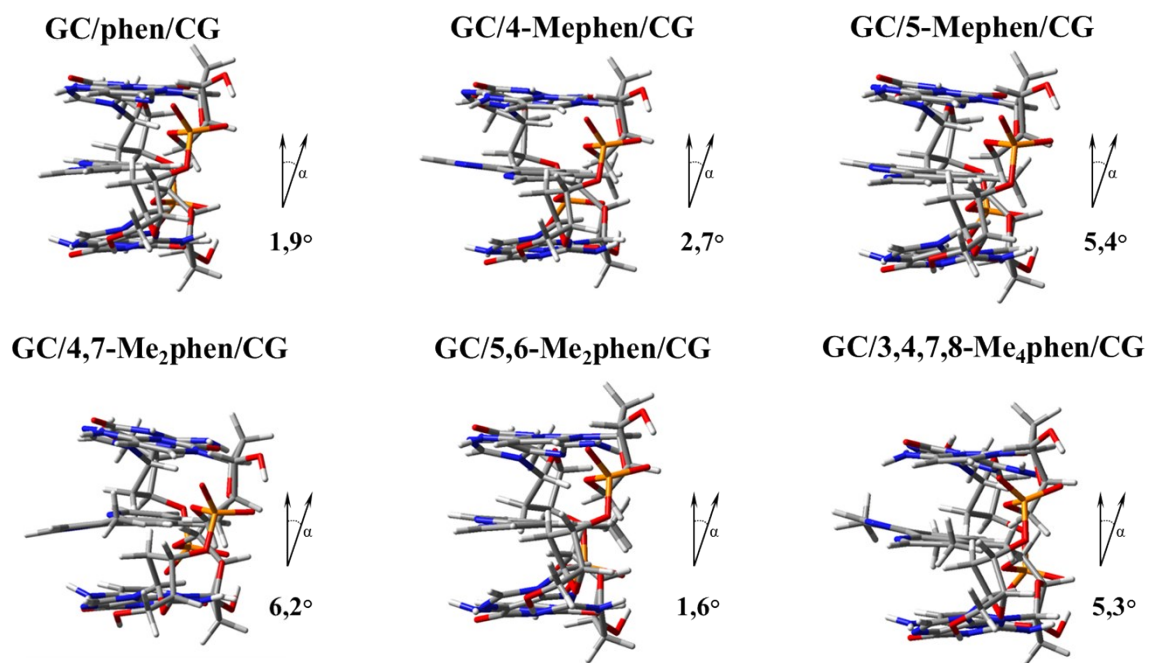
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## Roll Distortion

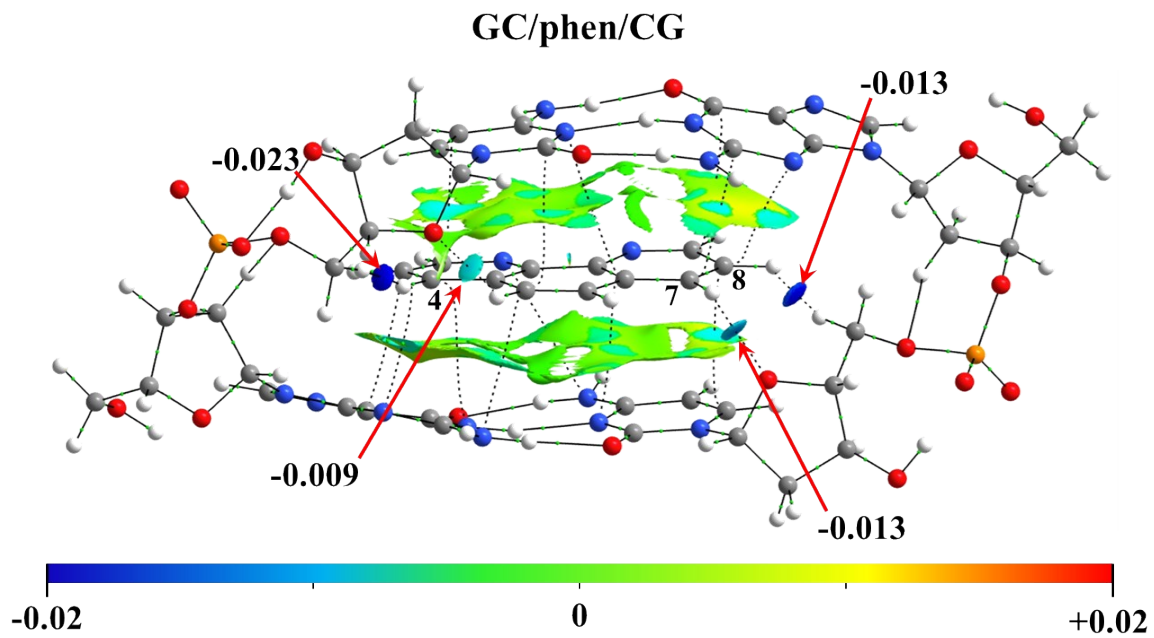


**Figure S1.** Definition of angle for Roll distortion between two base pairs

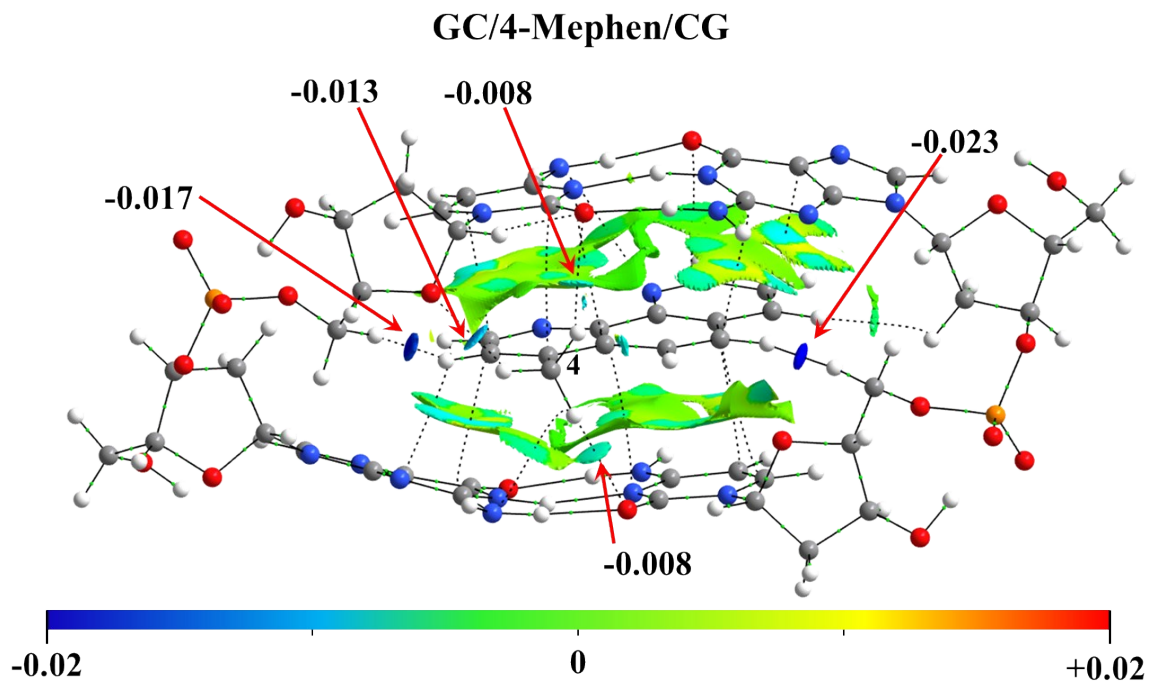
## Roll Distorsion (intercalation via Major Groove)



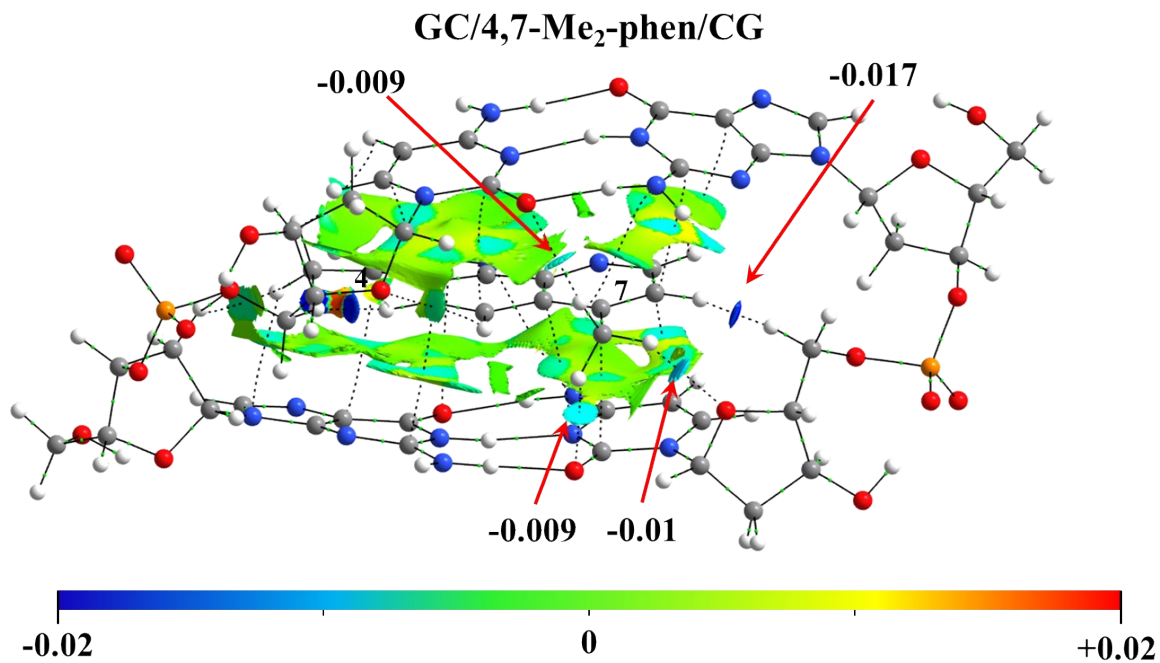
**Figure S2.** Roll distortion between GC/CG base pairs for the intercalation through the Major Groove of the studied systems.



**Figure S3.** Detailed NCI plot with gradient isosurfaces ( $s = 0.5$  a.u.) computed for phen intercalated between GC/CG base pairs via Major Groove.

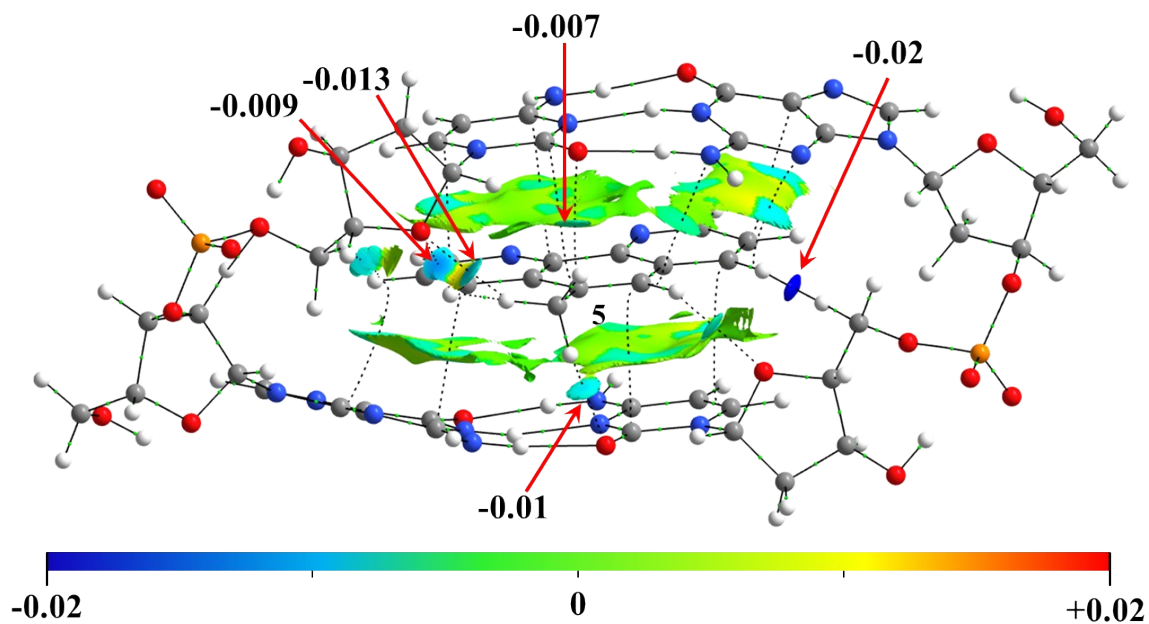


**Figure S4.** Detailed NCI plot with gradient isosurfaces ( $s = 0.5$  a.u.) computed for 4-Mephen intercalated between GC/CG base pairs via Major Groove.



**Figure S5.** Detailed NCI plot with gradient isosurfaces ( $s = 0.5$  a.u.) computed for 4,7-Me<sub>2</sub>phen intercalated between GC/CG base pairs via Major Groove.

### GC/5-Mephen/CG

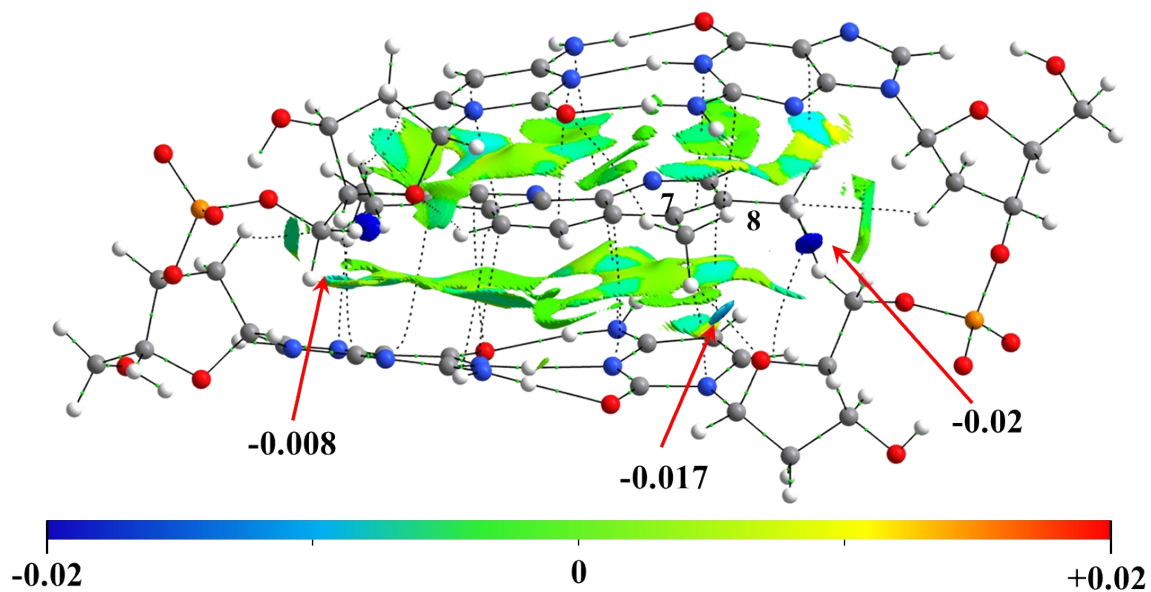


**Figure S6.** Detailed NCI plot with gradient isosurfaces ( $s = 0.5$  a.u.) computed for 5-Mephen intercalated between GC/CG base pairs via Major Groove.



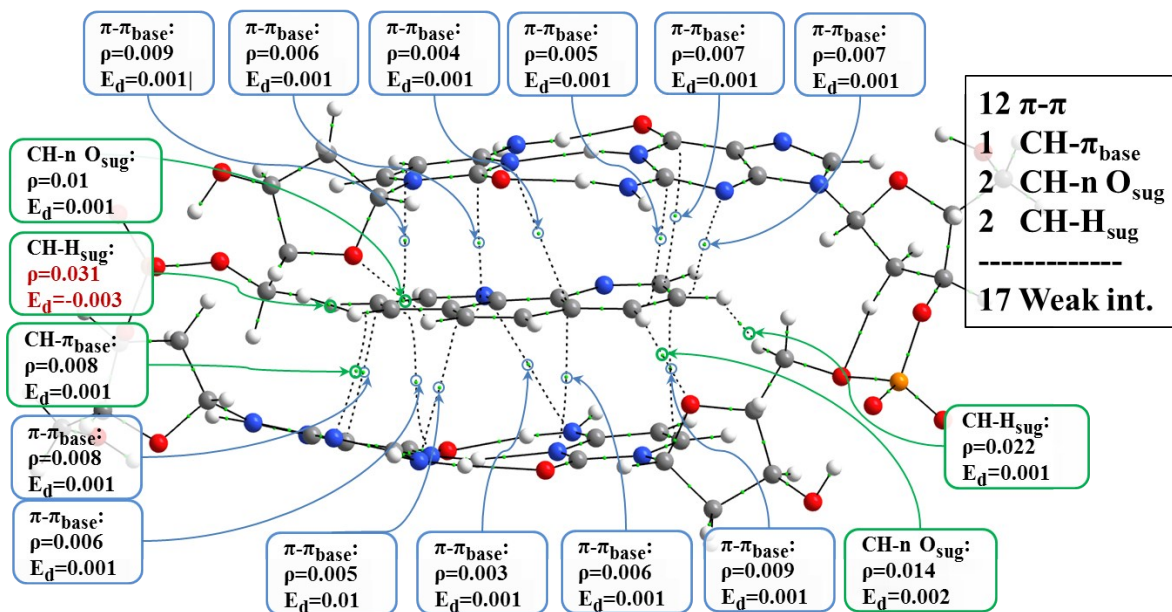


### GC/3,4,7,8-Me<sub>4</sub>phen/CG



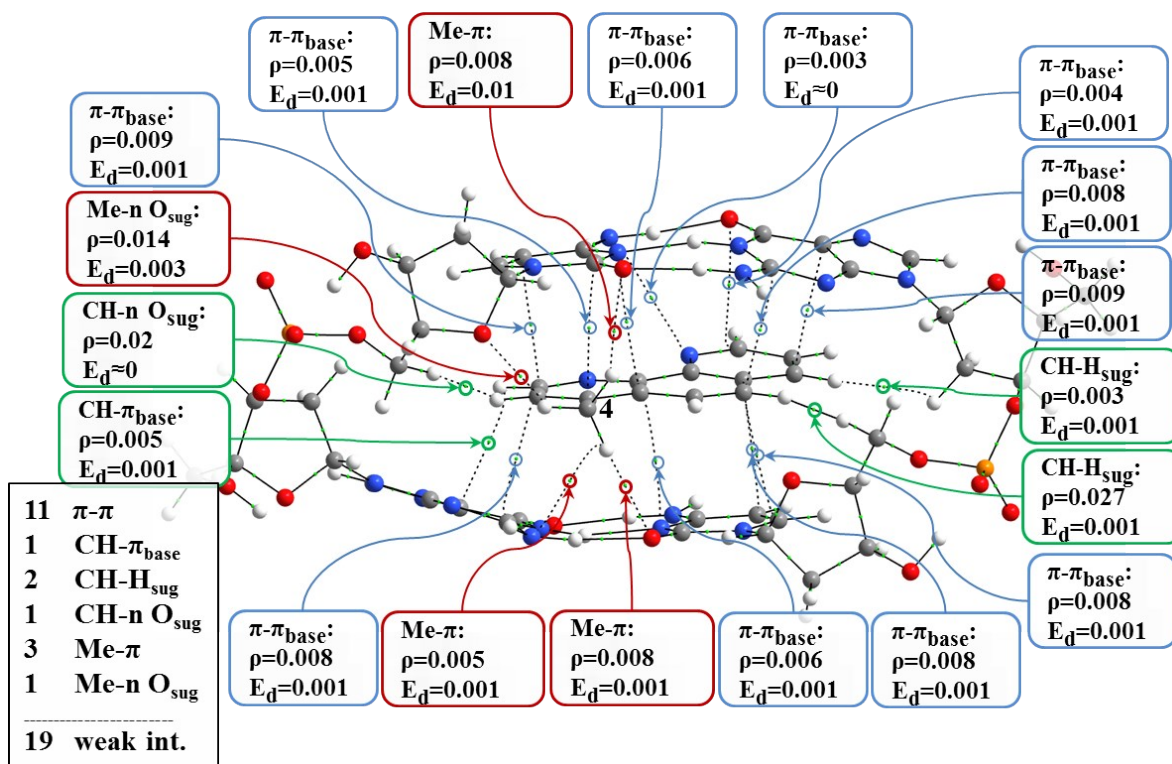
**Figure S8.** Detailed NCI plot with gradient isosurfaces ( $s = 0.5$  a.u.) computed for 3,4,7,8-Me<sub>4</sub>phen intercalated between GC/CG base pairs via Major Groove.

**QTAIM: GC/Phen/CG**  
**intercalation via Major Groove**

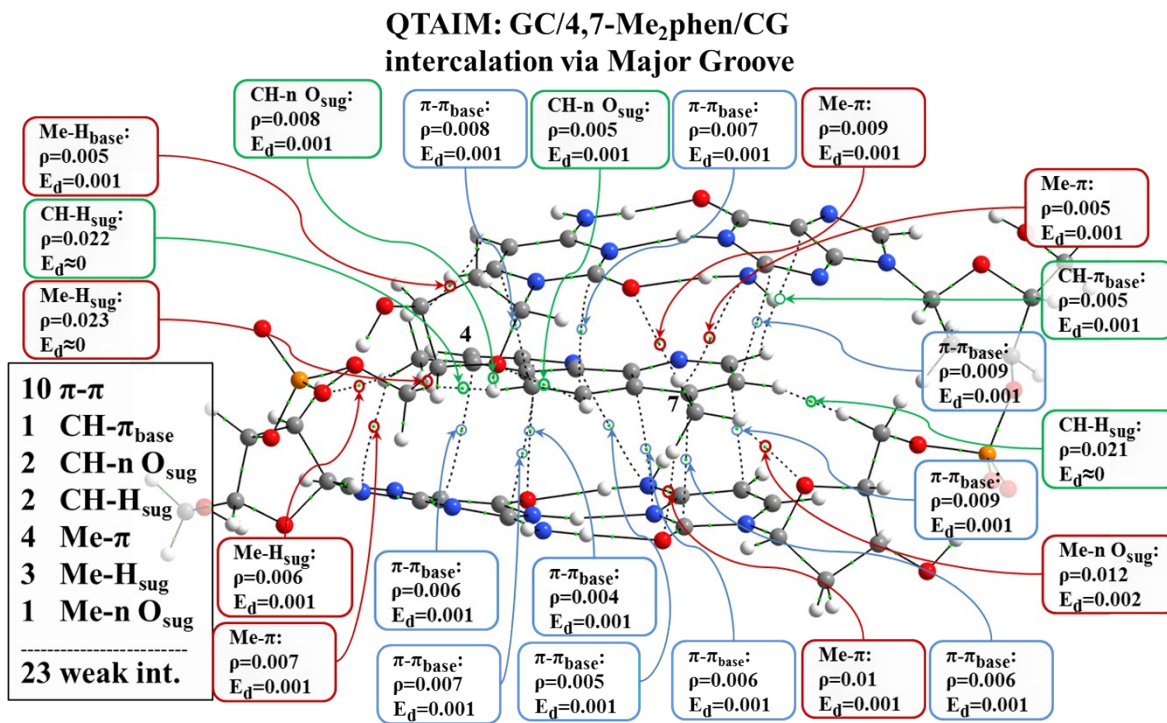


**Figure S9.** Complete bonding scheme from QTAIM topological analysis of  $\rho$  for phen, intercalated between GC/CG base pairs via Major Groove. For the considered interactions the corresponding BCPs,  $\rho$  (a.u.) and  $E_d$  (a.u.) are presented.

## QTAIM: GC/4-Mephen/CG intercalation via Major Groove

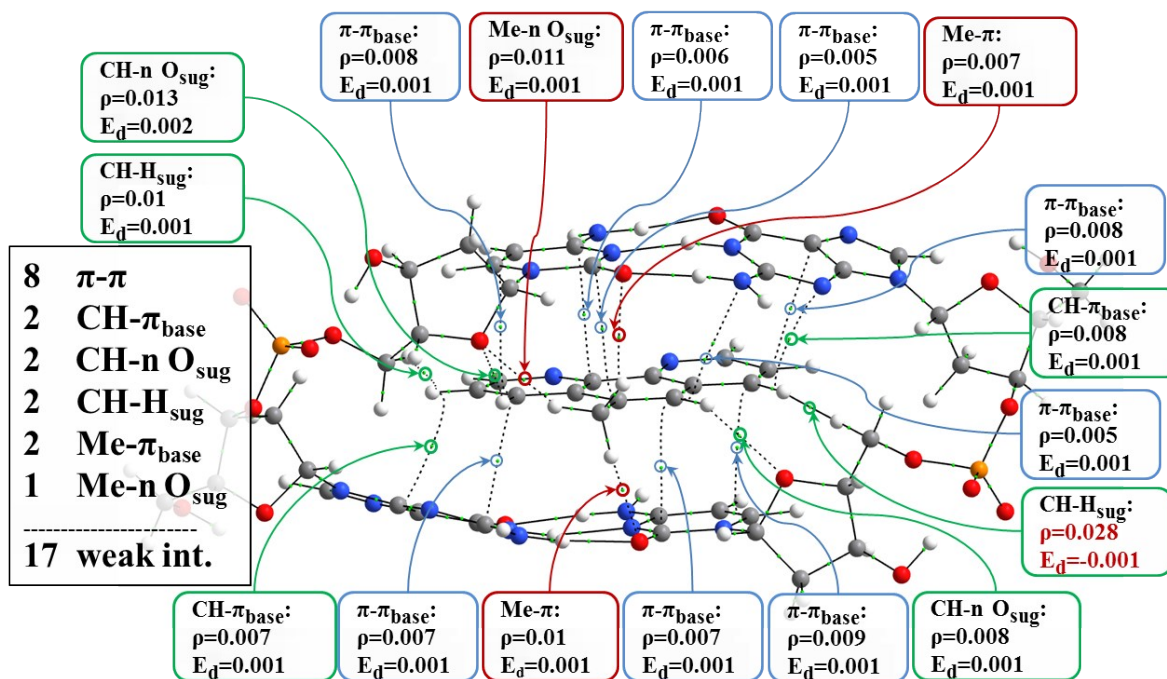


**Figure S10.** Complete bonding scheme from QTAIM topological analysis of  $\rho$  for 4-Mephen, between GC/CG base pairs via Major Groove. For the considered interactions the corresponding BCPs,  $\rho$  (a.u.) and  $E_d$  (a.u.) are presented.



**Figure S11.** Complete bonding scheme from QTAIM topological analysis of  $\rho$  for 4,7-Me<sub>2</sub>phen between GC/CG base pairs via Major Groove. For the considered interactions the corresponding BCPs,  $\rho$  (a.u.) and  $E_d$  (a.u.) are presented.

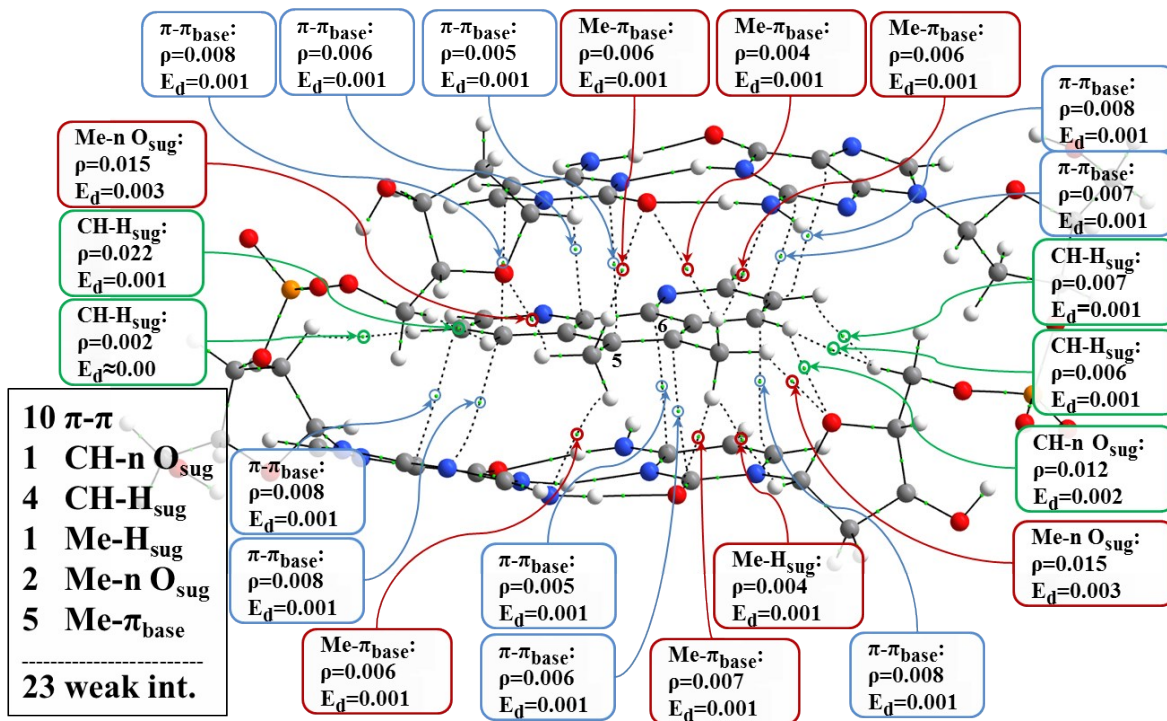
**QTAIM: GC/5-Mephen/CG**  
intercalation via Major Groove



**Figure S12.** Complete bonding scheme from QTAIM topological analysis of  $\rho$  for 5-Mephen between GC/CG base pairs via Major Groove. For the considered interactions the corresponding BCPs,  $\rho$  (a.u.) and  $E_d$  (a.u.) are presented.

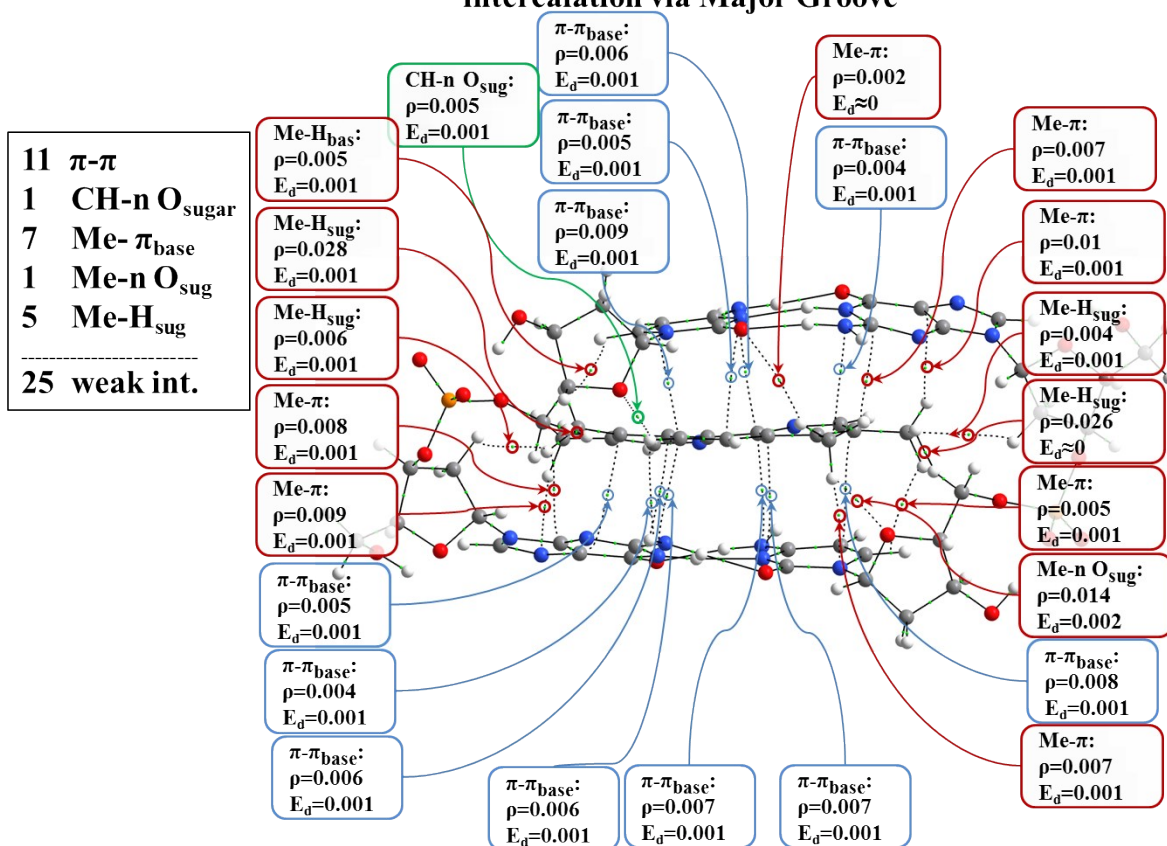


QTAIM: GC/5,6-Me<sub>2</sub>phen/CG  
intercalation via Major Groove



**Figure S13.** Complete bonding scheme from QTAIM topological analysis of  $\rho$  for 5,6-Me<sub>2</sub>phen between GC/CG base pairs via Major Groove. For the considered interactions the corresponding BCPs,  $\rho$  (a.u.) and  $E_d$  (a.u.) are presented.

QTAIM: GC/ 3,4,7,8-Me<sub>4</sub>phen /CG  
intercalation via Major Groove



**Figure S14.** Complete bonding scheme from QTAIM topological analysis of  $\rho$  for 3,4,7,8-Me<sub>4</sub>phen between GC/CG base pairs via Major Groove. For the considered interactions the corresponding BCPs,  $\rho$  (a.u.) and  $E_d$  (a.u.) are presented.



**Table S1.** Energies associated to the different kinds of weak interactions found in the studied systems,  $\Delta E_{wi}$ , between intercalators and GC/CG bps along with the total interaction energy,  $\Delta E_{int}$ , obtained with the EML approach. Results in kcal mol<sup>-1</sup>.

	phen	4-Mephen	5-Mephen	4,7-Me <sub>2</sub> phen	5,6-Me <sub>2</sub> phen	3,4,7,8-Me <sub>4</sub> phen
$\Delta E_{wi} \pi_{bps}-\pi$	-9.7	-9.9	-7.3	-9.2	-9.3	-8.1
$\Delta E_{wi} \pi_{bps}-CH$	-1.1	-0.6	-2.1	-0.5		
$\Delta E_{wi} \pi_{bps}-Me$		-3.4	-3.0	-5.0	-4.5	-8.0
$\Delta E_{wi} H_{sugar}-CH$	-9.9	-9.1	-6.9	-7.7	-5.9	
$\Delta E_{wi} H_{sugar}-Me$				-5.6	-0.6	-11.5
$\Delta E_{wi} O_{sugar}-CH$	-4.4		-3.9	-2.4	-2.2	-0.8
$\Delta E_{wi} O_{sugar}-Me$		-2.8	-2.1	-2.3	-5.9	-2.7
$\Delta E_{int}$ Total	-25.1	-25.8	-25.3	-32.7	-28.4	-31.1

## Cartesian Coordinates

### Cartesians coordinates for GC/phen/CG

146

C	2.86465500	1.55316200	-3.04458900
C	1.60190000	0.91606500	-3.16611500
C	1.57562300	-0.50015400	-3.26861700
N	2.73593600	-1.24384600	-3.31051000
C	3.90991300	-0.60655800	-3.23238900
C	4.01995700	0.80342700	-3.07490700
C	0.27765500	-1.17823800	-3.33298800
C	-0.90205600	-0.38924600	-3.40188600
C	-0.82291500	1.05025100	-3.32104100
C	0.37402800	1.67412400	-3.18661100
C	-2.14563000	-1.05717200	-3.54681600
C	-2.17985300	-2.43591100	-3.56376800
C	-0.96385400	-3.15565200	-3.41489000
N	0.22934300	-2.55581900	-3.32244100
H	-1.75659800	1.61408200	-3.35779700
H	0.44417900	2.76111300	-3.08147700
O	0.93203200	4.28699100	-1.25737800
C	0.37435100	3.77480400	-0.03073100
C	0.95896600	4.60183100	1.12172400
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C	1.91826900	5.32818900	-0.99180800
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O	5.71754700	7.04674100	-2.45399000
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C	4.79058500	1.69293500	-6.04394700
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C	2.19914300	2.71150500	-6.03880900
N	3.17686100	3.55531100	-5.56985100
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C	-0.94273700	-2.48876600	-6.64821300
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C	-5.46279600	-2.34661800	-4.92331500
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H	7.67144500	6.35346000	-2.16471700
H	7.33423300	4.13269800	-3.19917500
H	5.81899700	4.29732400	-2.31917200
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H	1.61055200	0.75125300	-6.63440600
H	0.12577300	2.56914100	-6.39111300
H	0.70708100	4.12628100	-5.83919100
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H	3.07254500	5.66538600	-2.83150000
H	1.41266700	6.28501800	-1.26703000
H	3.13848500	4.67077200	0.75450800
H	1.16389200	3.99740200	2.02142300
H	0.23844800	5.38009000	1.45346400
H	-0.73780600	3.84765600	-0.15555400
H	2.47797600	-2.11048500	-0.15014100
H	0.77876600	-2.43600100	0.00666900
H	3.41552900	0.24028200	0.02186900
H	2.84704700	2.67690700	0.00531500
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H	8.13661700	5.06985200	-5.80109700
H	2.71527000	7.23150800	0.33270700
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H	-4.42895700	0.22568500	-0.88380900
H	4.81231100	-1.22840100	-3.30890400
H	-0.96608300	-4.25347000	-3.36582200
H	5.00406800	1.26204000	-3.00509500
H	-3.12282500	-2.97423600	-3.68136200
H	2.90305600	2.64658500	-2.93722300
H	-3.06474300	-0.47177300	-3.66046900

### Cartesians coordinates for GC/4-Mephen/CG

149

N	1.43413600	1.58137000	3.49642100
C	0.94574500	0.29544200	3.40088400
C	-0.44462700	0.02231900	3.31003500
C	-1.35749300	1.12104300	3.39295100
C	-0.84588700	2.40314700	3.51822900
C	0.55804600	2.59284200	3.53670100
C	-0.89518500	-1.33629700	3.12684200
C	-0.01294400	-2.36071000	3.01823600
C	1.40446000	-2.13336300	3.13582400
C	1.89428200	-0.82376500	3.38101300
N	3.23347700	-0.58633800	3.60737500
C	4.08397800	-1.61747000	3.55232500
C	3.67968300	-2.94672500	3.24103900
C	2.34025800	-3.19799700	3.03788000
C	-2.82755200	0.89001300	3.35833000
C	-1.23690000	3.42018100	0.65240600
N	-1.37433800	4.66525800	1.21016800
C	-0.19877800	5.38137100	1.24640600
C	1.09059300	4.93635600	0.82355200
C	1.26552000	3.59081700	0.35073700
N	0.00318300	2.87205300	0.27303400
N	2.03904100	5.95432300	1.02338800
C	1.38643000	6.97561200	1.57136700
N	-0.02016300	6.68005300	1.74225000
C	-1.04381700	7.38720200	2.50764000
O	-1.39200500	8.60907000	1.78678300
C	-1.72377800	9.64692600	2.75997000
C	-1.51210200	9.02720700	4.17220800
C	-0.57292200	7.85103700	3.89427100
O	-2.85279100	8.60736200	4.51901300
P	-3.07460800	7.69963300	5.87105900
O	-2.38734600	8.26886000	7.09163900
C	-0.77274500	10.81273800	2.43709600
O	0.47691900	10.30376600	1.96248900
N	-2.37284500	2.67861600	0.40398700
O	2.25615100	2.95837800	0.03369000
O	-2.21488400	6.27124600	5.56813300
C	-2.89541000	5.24925700	4.83580000
C	-3.83706800	4.44770900	5.74989800
O	-3.57575300	3.04180900	5.46530900
C	-3.32268500	2.30301300	6.67305800
C	-3.73757800	3.20528700	7.84317600

C	-3.61911800	4.63323800	7.28085900
N	-1.86836900	1.95155200	6.71012500
C	-1.49119500	0.53846400	6.61511000
N	-0.15625900	0.20861700	6.63857700
C	0.81920900	1.17738300	6.66513000
C	0.45194300	2.57901700	6.67532700
C	-0.86900500	2.92448700	6.68436300
O	-2.39911200	-0.28328000	6.52136800
N	2.11536800	0.77257900	6.72368500
O	-4.62634000	5.46088200	7.85292400
O	-4.54244200	7.33760900	6.00945800
N	2.33515900	0.10385600	-0.00691800
C	1.20869800	-0.65392800	-0.01741300
C	1.25867900	-2.10049100	-0.06884000
C	0.08966900	-2.80607500	-0.09348300
N	-1.14450900	-2.15704100	-0.11173700
C	-1.18707500	-0.69492600	0.00000000
N	0.00000000	0.00000000	0.00000000
O	-2.29212900	-0.16600000	0.07731600
C	-2.43685900	-2.91175800	-0.07953600
O	-2.46524400	-3.69212100	1.12789400
C	-2.32201900	-5.11516300	0.84097200
C	-2.04014400	-5.22566600	-0.68665800
C	-2.56958300	-3.89479300	-1.25083200
C	-1.21092300	-5.62582600	1.77248800
O	-0.23290900	-6.38020100	1.05173100
P	-0.60971700	-7.99865900	0.72332300
O	-2.11542500	-8.10152600	0.55206200
O	-2.74849100	-6.31270300	-1.27098700
O	0.24372700	-8.32343600	-0.48071000
O	-0.15932200	-8.81119400	2.08002700
C	1.23082200	-8.79722700	2.47713100
C	1.18238500	-9.52897100	3.84985400
O	1.10715900	-8.49535400	4.87975700
C	1.07643500	-7.18840100	4.23163500
C	1.72139800	-7.39638100	2.85202400
C	2.45440800	-10.33055500	4.17927100
O	3.42938000	-9.47256600	4.77875000
N	1.79843400	-6.23961100	5.07743200
C	1.23434000	-5.03374200	5.51820800
C	2.31403400	-4.25639500	6.03763900
N	3.51481600	-4.98142000	5.94660200
C	3.21179700	-6.14240300	5.37147100
C	2.07981100	-2.89988800	6.45111600
N	0.67106900	-2.54738700	6.40464400
C	-0.33806300	-3.41309800	5.94035000
N	-0.08563000	-4.65895500	5.42032900
N	-1.64379800	-2.99621300	6.04220800
O	2.83918700	-2.00940300	6.78828700
H	-1.20066300	11.46751600	1.65430100
H	-0.50414500	11.41900500	3.31963500

H	-2.79510700	9.88564300	2.58004300
H	-1.14413200	9.73984600	4.93704900
H	0.47977300	8.20181400	3.88627000
H	-0.59408300	7.03399000	4.64481200
H	-1.98612500	6.77674800	2.52994900
H	1.79387600	7.93722900	1.85373400
H	0.04003000	1.84769600	0.00000000
H	-2.30290200	1.66252800	0.21550000
H	-2.07124300	4.59573600	4.45242300
H	-3.43571900	5.66218400	3.96061000
H	-4.90636200	4.59749400	5.46874600
H	-2.61591900	5.07327300	7.51001000
H	-3.13111100	3.03903200	8.74926700
H	-4.78539400	2.99812500	8.14787500
H	-3.91076500	1.35519700	6.56236000
H	2.86517400	1.40810600	6.48319900
H	2.36528800	-0.23661500	6.69747900
H	1.22962600	3.33842400	6.65928600
H	-1.18557900	3.97981900	6.67071200
H	2.23322300	-11.15195600	4.88709100
H	2.96111200	-10.73884900	3.28746900
H	0.24550800	-10.11833000	3.96093100
H	1.84019200	-9.30773300	1.70485000
H	2.82956100	-7.38376700	2.90127500
H	1.45541800	-6.59551300	2.13246500
H	-0.00871600	-6.90274600	4.18679300
H	3.88472700	-6.96105900	5.15087500
H	0.40694800	-1.54562800	6.64286800
H	-1.87614400	-2.01280700	6.27013400
H	-2.37268600	-3.55959200	5.62745400
H	-0.62894800	-4.76373900	2.19249500
H	-1.62822200	-6.19995300	2.62365100
H	-3.31183000	-5.55658900	1.10596500
H	-0.94813000	-5.34584700	-0.90124700
H	-2.03670400	-3.55928800	-2.15624500
H	-3.63163900	-4.00230800	-1.55738200
H	-3.27273500	-2.17327400	0.03048500
H	3.24521600	-0.31016100	0.12101900
H	2.29382400	1.14372800	0.05007800
H	2.21815400	-2.60971700	-0.06079900
H	0.08646800	-3.90832600	-0.09946700
H	-4.92188900	6.18172500	7.12185700
H	2.95840100	-8.89454400	5.44925200
H	-2.81651400	-7.09509100	-0.54686100
H	0.28054900	9.56396100	1.31518900
H	-3.25119200	3.00436000	0.78563800
H	-0.35905200	-3.38947500	2.84771400
H	-1.96937000	-1.52134300	3.05579800
H	-3.13705300	0.15390800	4.12010500
H	-3.40388100	1.80530100	3.57173000
H	-3.14941800	0.50652000	2.37611600

H	5.13674900	-1.39592300	3.77182300
H	0.98357400	3.60464400	3.58723700
H	4.42246700	-3.74161700	3.20810000
H	-1.50850700	3.26932800	3.60992900
H	1.98289900	-4.20420000	2.82112800

### Cartesians coordinates for GC/5-Mephen/CG

149

C	-2.80662900	1.67374900	2.99482600
C	-1.59858100	0.93873300	3.14206100
C	-1.68925300	-0.47013000	3.28455600
N	-2.90615700	-1.11624800	3.34876200
C	-4.02309900	-0.38872700	3.24925200
C	-4.01766100	1.02115000	3.04607700
C	-0.44986700	-1.24713200	3.35916400
C	0.79766400	-0.56605400	3.37728700
C	0.84151000	0.88337400	3.26974900
C	-0.31821000	1.59029200	3.13912600
C	1.97385300	-1.35101000	3.50159600
C	1.88923500	-2.72574800	3.55999600
C	0.60627600	-3.33142100	3.48240600
N	-0.52649000	-2.62355500	3.40396100
C	2.15077000	1.59830100	3.28031500
H	-0.30549200	2.67727900	3.02235300
O	-0.98052400	4.31450700	1.19423700
C	-0.36765400	3.77574000	0.00670000
C	-0.89498000	4.57740100	-1.19027600
C	-2.17614200	5.25928100	-0.67476400
C	-1.94256000	5.36004400	0.85998800
N	-0.73772400	2.32861900	-0.06618000
C	0.33630600	1.33345500	0.00000000
N	0.00000000	0.00000000	0.00000000
C	-1.31432800	-0.40380000	-0.00747100
C	-2.38033900	0.57598500	-0.04225600
C	-2.06529300	1.90549500	-0.04808900
O	1.48997500	1.75264200	0.04027400
N	-1.56304500	-1.73918600	-0.01191300
C	-3.16647900	5.09789800	1.75022700
O	-4.38234500	5.20615300	1.00822500
P	-4.97441900	6.76761000	0.71883700
O	-3.77644700	7.68428300	0.55835900
O	-2.29677800	6.54292200	-1.27731200
O	-5.87733800	6.56430400	-0.47639800
O	-5.79298700	7.17423600	2.08560200



C	-6.92628900	6.37415600	2.49410300
C	-7.26174000	6.97953300	3.88953600
O	-6.59366700	6.14258200	4.88583800
C	-5.82003400	5.12218700	4.18303800
C	-6.53459100	4.93384000	2.83582400
C	-8.75406500	6.91514800	4.25760000
O	-9.06664400	5.62477900	4.79075600
N	-5.78037800	3.91826800	5.00856000
C	-4.57997200	3.33450900	5.43759600
C	-4.92406100	2.04467700	5.94559600
N	-6.31318800	1.84935000	5.85721000
C	-6.81408800	2.94821100	5.29850000
C	-3.88663500	1.14222500	6.36257300
N	-2.57084900	1.75628200	6.31110600
C	-2.33274800	3.06034900	5.83412400
N	-3.31860600	3.87355700	5.33073700
O	-3.91411800	-0.02532200	6.70902200
N	-1.04987900	3.54501800	5.89114200
N	-1.61261200	-1.73226000	6.68038700
C	-0.34967900	-1.23521400	6.63340100
N	-0.20071600	0.13012200	6.57631700
C	1.04330700	0.71472100	6.54215700
N	2.22598700	-0.15113400	6.62058900
C	2.06020200	-1.53429200	6.65770000
C	0.81538700	-2.09555500	6.68147900
C	3.57655100	0.47862200	6.50289800
O	4.20895800	-0.08105000	5.33400900
C	5.40516100	-0.83513100	5.69079300
C	5.40237700	-0.96551400	7.24079200
C	4.47936500	0.17761100	7.70460400
C	5.31148200	-2.16512300	4.92763800
O	5.92912300	-3.22350100	5.66016500
P	7.62592000	-3.25389900	5.75043600
O	8.09047400	-1.81576300	5.84424500
O	6.69906100	-0.77819600	7.79645200
O	1.23693100	1.92289000	6.45697100
O	8.13856600	-3.88787100	4.32412800
C	7.69612000	-5.20134200	3.91420900
C	8.26676800	-5.28956800	2.46635100
O	7.19371900	-4.86568300	1.56615200
C	6.05902900	-4.44012300	2.38394000
C	6.18275400	-5.25777700	3.67885100
N	4.83114900	-4.66956500	1.63083000
C	4.01759100	-3.62549000	1.16713100
C	2.80098700	-4.23229500	0.72953900
N	2.87814200	-5.62684700	0.88618200
C	4.07086800	-5.88220200	1.41757900
C	1.70706000	-3.40771400	0.29510500
N	2.06340100	-1.99952300	0.25387400
C	3.31505100	-1.49717300	0.66111800
N	4.31223700	-2.28212300	1.18513800

N	3.55160200	-0.15326100	0.51157100
O	0.55632800	-3.67263500	-0.00313100
C	8.61207800	-6.71916300	2.01773100
O	7.42142100	-7.39583200	1.60292300
O	7.83807300	-4.17693800	6.92804000
H	9.32035600	-6.70739000	1.16750400
H	9.01727100	-7.34894100	2.82874700
H	9.09122000	-4.56032600	2.31006900
H	8.08869300	-5.96264000	4.61531700
H	5.86261800	-6.31167900	3.54264500
H	5.55863900	-4.86987900	4.50737800
H	6.19987400	-3.33274300	2.54192500
H	4.48163700	-6.85127300	1.66197000
H	1.29759900	-1.30782700	0.00000000
H	2.79248000	0.50399900	0.26018600
H	4.25496900	-2.49925000	4.83567800
H	5.73403400	-2.07785800	3.90250700
H	6.25955200	-0.20945600	5.32997600
H	5.02905600	-1.96242500	7.57795300
H	3.90904800	-0.06655300	8.61697000
H	5.08631900	1.06893200	7.97438900
H	3.43714500	1.56729200	6.27304500
H	-1.79409900	-2.71099500	6.50701200
H	-2.44287900	-1.10586200	6.63815500
H	0.68704100	-3.17379900	6.71576000
H	2.97063300	-2.14972700	6.66454700
H	-9.00781900	7.67657700	5.01945800
H	-9.42670300	7.02306500	3.38895300
H	-6.81661900	7.99147000	4.00934300
H	-7.73510200	6.46944600	1.74319400
H	-7.44459400	4.30582200	2.92727800
H	-5.90433100	4.42020900	2.08181300
H	-4.78337400	5.54666800	4.08806500
H	-7.85350600	3.15836400	5.08636200
H	-1.73549100	1.14652300	6.55445100
H	-0.25188800	2.93446600	6.13934400
H	-0.84253600	4.44723100	5.48734900
H	-3.16721700	4.03718300	2.11144100
H	-3.16736600	5.75745200	2.64207900
H	-1.43783000	6.31826000	1.13144300
H	-3.08891900	4.66433300	-0.92107700
H	-1.06256400	3.95202800	-2.08347000
H	-0.15639000	5.34438500	-1.50808300
H	0.73753400	3.84727200	0.18039800
H	-2.48804400	-2.09916700	0.17437200
H	-0.79007000	-2.43491200	0.02800000
H	-3.41592900	0.24720300	-0.03604000
H	-2.84227100	2.68382500	-0.03713100
H	7.43289000	-0.89805200	7.02803900
H	-8.33748000	5.37379600	5.43069100
H	-2.66394600	7.23614700	-0.54854900

H	6.89627200	-6.76527900	1.02850600
H	4.42266900	0.23594700	0.84372000
H	-4.97362800	-0.93080400	3.34324300
H	0.50396400	-4.42561100	3.47633200
H	-4.96165200	1.55408600	2.95443400
H	2.77552600	-3.35049300	3.64447700
H	-2.75526600	2.76155300	2.84536400
H	2.94643200	-0.84215700	3.56168700
H	2.14122400	2.43591900	3.99529500
H	3.00098600	0.95615100	3.56498000
H	2.36963500	2.01707100	2.28307200

**Cartesians coordinates for GC/4,7-Me<sub>2</sub>phen/CG**

152

C	-0.95351100	-0.99086000	0.00000000
N	-0.51691700	-2.38843200	-0.05036300
C	0.84569600	-2.67680600	0.03643700
C	1.77790800	-1.67963600	0.05969100
C	1.34195600	-0.29779800	0.02841300
N	0.00000000	0.00000000	0.00000000
C	-1.56252600	-3.45845000	-0.01834800
O	-1.44746200	-4.16275400	1.23070300
C	-0.91451800	-5.50537000	1.03302600
C	-0.55127700	-5.61564200	-0.47734400
C	-1.37628400	-4.49481700	-1.13483200
C	0.25910300	-5.64635400	2.01621400
O	1.41254700	-6.18694400	1.36695900
P	1.45079000	-7.86613700	1.14740800
O	0.02209600	-8.34130500	0.95035800
O	-0.93708000	-6.87620600	-1.01470000
N	2.22431300	0.73589200	-0.01852900
O	-2.16300600	-0.77876300	0.03954400
O	2.03724500	-8.45320300	2.56612300
C	3.37211500	-8.07899300	2.98014500
C	3.43455400	-8.65767000	4.42378200
O	3.09797100	-7.56548300	5.33347800
C	2.79657800	-6.37390300	4.54401500
C	3.52592600	-6.57305400	3.20689300
N	3.24703600	-5.20399000	5.29410900
C	2.38613300	-4.17239800	5.69248400
C	3.22403700	-3.10551800	6.13876700
N	4.57421400	-3.48591900	6.04920300
C	4.58663600	-4.71655300	5.54463000
N	1.01019000	-4.17386700	5.63102500
C	0.44246200	-3.01918200	6.10336300
N	1.18829100	-1.89123700	6.49553700
C	2.64186500	-1.85013900	6.52538800

O	3.13573200	-0.78468200	6.84731000
N	-0.92871900	-2.96853400	6.25330000
C	4.83817600	-9.11815500	4.85521300
O	5.58685700	-8.00281300	5.34646700
O	2.40234400	-8.04635300	-0.01354400
O	-2.35661700	-0.47860900	6.36649900
C	-1.69281300	0.54621000	6.48592400
N	-2.41845000	1.82309700	6.50523700
C	-1.69922400	3.01575800	6.56505100
C	-0.33877300	3.01677400	6.68206000
C	0.36831000	1.75200200	6.68403300
N	-0.32344800	0.56709300	6.61531700
C	-3.89510300	1.80995800	6.26917900
O	-4.13436500	2.41880300	4.98563100
C	-4.86194300	3.67504100	5.12112600
C	-4.89560700	3.99783800	6.64316900
C	-4.66573900	2.62884500	7.31184600
C	-4.12416800	4.68568000	4.22946100
O	-3.99907100	5.95908700	4.86560600
P	-5.36742100	6.95652200	4.91206000
O	-5.07822300	7.86492000	6.08540400
O	-6.15933200	4.50927500	7.04872300
N	1.72124700	1.68742800	6.77287400
O	-5.38118900	7.74842100	3.47147300
C	-4.27474800	8.60979000	3.11866100
C	-4.59557100	8.95180100	1.63250200
O	-3.84220700	8.00424100	0.81044000
C	-3.17825000	7.05788800	1.70567800
C	-2.95417000	7.84221400	3.00861200
N	-1.95837600	6.58417900	1.06243700
C	-1.72768000	5.22666600	0.79415500
C	-0.36216500	5.12578700	0.38978300
N	0.23291000	6.39867800	0.39398700
C	-0.70459400	7.25432900	0.79557900
N	-2.63052400	4.19949200	0.93747800
C	-2.13139600	2.97925900	0.54820600
N	-0.79009400	2.77498000	0.17201700
C	0.20379600	3.83376500	0.11035000
N	-2.98790100	1.90891200	0.50368200
O	1.34066300	3.47825800	-0.14177600
C	-4.09725900	10.33752400	1.18892300
O	-2.70710600	10.26797200	0.85702200
O	-6.59135300	6.06282000	4.99456600
C	-1.18181500	2.45535800	3.51006900
C	0.16899800	2.95021100	3.42489900
C	1.22692500	2.03350800	3.18442300
C	0.94295600	0.59312400	3.21919300
C	-0.40498700	0.15598000	3.28333600
C	-1.45943100	1.13168400	3.40880700
N	2.50778300	2.45469500	2.90193300
C	2.76137200	3.76994900	2.91899200

C	1.78997100	4.74229600	3.26684900
C	0.48961700	4.33912300	3.52722400
C	-0.66420500	-1.25038300	3.23132100
C	0.41180500	-2.12197600	3.17952600
C	1.73044800	-1.60289200	3.19768800
N	2.00026700	-0.29227100	3.19716500
C	-2.06053200	-1.76602900	3.21554300
C	-0.53072900	5.34943800	3.93111700
H	4.77655900	-9.87582600	5.65939700
H	5.44751200	-9.51168200	4.02304400
H	2.64663100	-9.42588900	4.58564300
H	4.10815600	-8.51638900	2.27642900
H	4.60165800	-6.30818600	3.27037400
H	3.12154200	-5.92488300	2.40201900
H	1.67764700	-6.35403500	4.45165700
H	5.45250000	-5.33400800	5.34455300
H	0.66922800	-0.99026200	6.70272400
H	-1.40659200	-2.05611100	6.36221700
H	0.59462300	-4.63864500	2.37073100
H	-0.02765400	-6.24119000	2.90635600
H	-1.75766100	-6.18514700	1.30107600
H	0.54351500	-5.46589300	-0.65557600
H	-0.90262400	-4.07332700	-2.03725400
H	-2.35772900	-4.88883100	-1.47411500
H	-2.56871500	-2.96542800	0.01933100
H	3.18221400	0.60663000	0.28510500
H	1.89325000	1.72220700	-0.01112300
H	2.83964300	-1.90563400	0.12162900
H	1.13897500	-3.73758500	0.08592400
H	-4.65027900	10.69123800	0.29800600
H	-4.15131100	11.10017100	1.98515600
H	-5.66563800	8.76519700	1.39560700
H	-4.25322400	9.48185900	3.80039600
H	-2.10650400	8.55307900	2.92972600
H	-2.71387800	7.19044500	3.87205400
H	-3.89752600	6.19984600	1.82066900
H	-0.60843000	8.32514200	0.90161900
H	-0.45866100	1.77886700	0.00000000
H	-2.65050700	0.95129800	0.30185300
H	-3.93720800	2.01732600	0.82982300
H	-3.05675500	4.36902500	4.06716600
H	-4.60128000	4.77151500	3.23126400
H	-5.88517900	3.45792500	4.72901200
H	-4.10506100	4.73323900	6.93106100
H	-4.14032100	2.69811000	8.27902700
H	-5.64161100	2.15131000	7.54519600
H	-4.22250700	0.74405400	6.15494700
H	2.29242500	2.51523300	6.71310500
H	2.22852500	0.77620800	6.75989000
H	0.21867800	3.94623000	6.74406300
H	-2.27157700	3.95388500	6.51820600

H	-0.84693700	-7.61041700	-0.24349300
H	-2.56534500	9.44047500	0.31025400
H	-6.62715600	4.97914800	6.20770500
H	4.98159800	-7.46290300	5.93587000
H	-1.48081200	-3.71428000	5.84957600
H	-0.42319600	6.28140000	3.35550400
H	-1.56891600	4.99646100	3.78590600
H	-0.42412300	5.61429600	4.99219700
H	-1.99277300	3.18595100	3.63814100
H	-2.49287100	0.77997800	3.44406900
H	-2.64524000	-1.31184200	2.39639400
H	-2.10602000	-2.85466500	3.05105500
H	-2.58315200	-1.54006400	4.15981200
H	3.78022700	4.07549500	2.64723600
H	2.59563800	-2.27941500	3.21000600
H	2.07000000	5.79348700	3.28752200
H	0.26015000	-3.20423500	3.11594300

#### Cartesians coordinates for GC/5,6-Me<sub>2</sub>phen/CG

152

C	1.22522500	0.62549100	0.00000000
N	2.43086000	-0.19863600	0.14549800
C	2.31208100	-1.58755000	0.13313000
C	1.08747100	-2.19100300	0.09859700
C	-0.10505700	-1.36929200	0.04952100
N	0.00000000	0.00000000	0.00000000
C	3.76088700	0.48294000	0.17657400
O	4.46952800	0.11567200	-1.02220800
C	5.64346600	-0.69134800	-0.71743800
C	5.56257400	-1.03455600	0.79764200
C	4.62487100	0.04637800	1.36727800
C	5.58657300	-1.89213600	-1.67500600
O	5.94274500	-3.10114400	-1.00310200
P	7.59822900	-3.37731300	-0.75620900
O	7.60428500	-4.38541500	0.37048600
O	6.83652800	-0.93836200	1.42649400
N	-1.35155300	-1.90742200	0.09238100
O	1.37773900	1.83896300	-0.09602200
O	8.12334000	-3.99827800	-2.18562600
C	7.58054000	-5.26586000	-2.62425600
C	8.19475700	-5.41459600	-4.04595400
O	7.19004200	-4.94565800	-4.99710800
C	6.02174600	-4.48042700	-4.25736900
C	6.07636200	-5.20348000	-2.90269900
N	4.82665200	-4.79667200	-5.03895600

C	3.93299400	-3.81982800	-5.50316500
C	2.74331100	-4.51702000	-5.87816700
N	2.91376000	-5.89871300	-5.68606800
C	4.13509100	-6.06101800	-5.18608900
C	1.57719200	-3.77943400	-6.27769300
N	1.83702300	-2.35392200	-6.37351600
C	3.07530500	-1.76154600	-6.05932100
N	4.14051900	-2.46033000	-5.54648900
N	3.22763600	-0.41925500	-6.31527600
O	0.43260600	-4.12812800	-6.50638200
C	8.47771200	-6.87087600	-4.45542900
O	7.28275800	-7.47395100	-4.95995500
O	8.24858600	-2.03083900	-0.50489600
N	-0.96625100	3.39224600	-0.64770700
C	-2.23067300	2.86175400	-0.71038500
N	-3.24549800	3.63831700	-1.21499100
C	-4.48894900	3.06637900	-1.08373700
C	-4.78683500	1.77351400	-0.55298700
C	-3.71744400	0.90036100	-0.15460800
N	-2.42120900	1.55101600	-0.23068500
N	-6.17286400	1.54583100	-0.59250600
C	-6.71731200	2.62718100	-1.14326200
N	-5.71539300	3.61264600	-1.49091700
O	-3.70563900	-0.26759800	0.19123800
C	-5.82199500	4.81285900	-2.31353600
O	-6.33380300	5.89942600	-1.48085600
C	-7.09061400	6.81375700	-2.33549500
C	-7.10146900	6.18703400	-3.76222600
C	-6.81861900	4.70755300	-3.47822300
C	-8.48005000	6.90075600	-1.68262100
O	-8.84201700	5.62430800	-1.14670300
O	-5.98197200	6.85508300	-4.38507500
P	-5.47058300	6.39423400	-5.87643700
O	-6.57510900	6.33073300	-6.90528500
O	-5.07470100	4.74434500	-5.74035200
C	-3.83640900	4.39968000	-5.12067200
C	-2.64897100	4.75855300	-6.02609500
O	-1.58340900	3.82935300	-5.67579200
C	-0.98521900	3.25024200	-6.85337000
C	-1.62187800	3.92764400	-8.07303500
C	-2.91545800	4.58031100	-7.54753500
N	-1.24567400	1.77962400	-6.80123200
C	-0.10013400	0.86494500	-6.71614100
N	-0.34638000	-0.48401900	-6.60645900
C	-1.62740400	-0.97362000	-6.51536900
C	-2.75987200	-0.07032100	-6.55419800
C	-2.53726800	1.27101400	-6.67884500
O	-3.12332800	5.82485700	-8.20597500
O	1.02111700	1.35959100	-6.76203000
N	-1.78765200	-2.31988600	-6.43277500
O	-4.18704600	7.12744700	-6.20088500

C	-3.50912400	0.97603800	-3.45516700
C	-3.66083400	-0.42238000	-3.24230200
N	-2.62269700	-1.26089300	-3.16744700
C	-1.34501500	-0.74766900	-3.26545500
C	-1.10328700	0.64179700	-3.42213300
C	-2.23604900	1.49368800	-3.54089400
C	0.25249400	1.15362400	-3.44887100
C	1.32027700	0.30386400	-3.28905200
C	1.10842600	-1.12411900	-3.16255900
C	-0.20515400	-1.66216100	-3.19499500
N	-0.44032300	-3.02144100	-3.15597200
C	0.60060800	-3.85340300	-3.05378100
C	1.94366600	-3.39682100	-2.94486200
C	2.18296700	-2.04218200	-3.00365900
C	0.48153600	2.61640600	-3.65016700
H	-8.48462900	7.63910300	-0.85833400
H	-9.28757500	7.13766100	-2.39690100
H	-6.52717800	7.77201700	-2.31720000
H	-8.02156400	6.38054200	-4.34688400
H	-7.75972500	4.19924600	-3.18120200
H	-6.43386900	4.12443200	-4.33730900
H	-4.79179100	5.13853000	-2.63697700
H	-7.76772100	2.81168200	-1.31618300
H	-1.56411600	0.96679900	0.00000000
H	-0.14596200	2.80565000	-0.41166200
H	-3.91479400	3.30008100	-4.98098200
H	-3.74031400	4.86883300	-4.11569900
H	-2.23712700	5.77321200	-5.79179800
H	-3.81037500	3.94343700	-7.74744900
H	-1.79675100	3.22791300	-8.90783000
H	-0.94643300	4.70684500	-8.48772200
H	0.11780600	3.41552900	-6.74010200
H	-2.66834900	-2.72167600	-6.14363500
H	-0.96922100	-2.96168600	-6.39818000
H	-3.76744000	-0.46598400	-6.46380600
H	-3.36462700	1.99389300	-6.68646800
H	9.25102000	-6.91682800	-5.24564100
H	8.77431300	-7.51606700	-3.61021200
H	9.06623300	-4.73732700	-4.18337100
H	7.88135100	-6.05955500	-1.91053700
H	5.66395300	-6.23221600	-2.95634900
H	5.47006800	-4.69535200	-2.12471400
H	6.14106900	-3.36665700	-4.18518000
H	4.61921700	-6.99447100	-4.93054000
H	1.01901500	-1.71930600	-6.61123300
H	2.40751000	0.18184400	-6.51549500
H	4.07257500	0.04352500	-6.00983100
H	4.53827500	-2.07338400	-2.01653100
H	6.21368800	-1.72164100	-2.57325900
H	6.51452400	-0.02876700	-0.94089100
H	5.15894800	-2.06170000	0.97410900



H	4.02776700	-0.30280800	2.22634500
H	5.22028800	0.90070700	1.75508500
H	3.59019600	1.58784500	0.08943100
H	-1.50270800	-2.88930600	-0.09206700
H	-2.20139100	-1.30774200	0.06067500
H	0.99679700	-3.27372300	0.08785000
H	3.24180000	-2.17487800	0.15481100
H	-3.30325500	6.58441900	-7.47773900
H	6.84376900	-6.81616900	-5.57590000
H	7.59442800	-1.10642200	0.69285300
H	-8.04600900	5.26068800	-0.65923200
H	-0.79313100	4.30495900	-1.04476200
C	2.70959300	0.85068300	-3.23815700
H	0.37677400	-4.92881200	-3.06744300
H	-4.65995500	-0.86186800	-3.11895000
H	2.75025400	-4.11757100	-2.83471000
H	-4.39226700	1.60627300	-3.52325100
H	3.20990700	-1.65236700	-2.92874500
H	-2.06925600	2.56797500	-3.70406900
H	1.13637900	2.79154900	-4.51980700
H	-0.44462700	3.18457900	-3.84362800
H	0.97149200	3.06633300	-2.77479500
H	2.82740300	1.53781200	-2.38229300
H	3.48527500	0.07998700	-3.10745800
H	2.95449900	1.42004000	-4.14461400

### Cartesians coordinates for GC/3,4,7,8-Me,phen/CG

158

C	1.79310200	-1.32894500	3.36583500
C	1.25306600	-2.65394600	3.17058400
C	-0.14345800	-2.79219200	2.96610700
C	-1.01571500	-1.62900200	3.14428200
C	-0.44431400	-0.34383800	3.32310900
C	0.99349000	-0.23309600	3.40588300
N	-2.37999000	-1.82928800	3.14642100
C	-3.17347600	-0.76474400	3.26927400
C	-2.69080100	0.57630600	3.35340900
C	-1.31538200	0.78920100	3.41143300
C	2.06279300	-3.83181600	3.14124400
C	1.47434600	-5.04589100	2.79388600
C	0.08014300	-5.05980400	2.48373600
N	-0.71041400	-3.98998800	2.58732800
C	2.23035500	-6.32507600	2.68931900
N	3.45009900	0.28148200	0.86599000
C	3.49909200	-1.06443000	0.58758300

N	2.33485400	-1.68571900	0.10116000
C	2.22303700	-3.11119000	-0.16273600
C	3.48153300	-3.78895000	0.00058800
C	4.60739000	-3.07457800	0.51183400
N	4.66386400	-1.74246700	0.84984100
N	3.82295500	-5.13719800	-0.19926100
C	5.08942400	-5.26953100	0.19092700
N	5.64271500	-4.01313600	0.64395000
C	6.85129100	-3.73784300	1.41873200
O	8.01398900	-3.95815900	0.56449200
C	9.11827600	-4.42579700	1.40261400
C	8.55953300	-4.57027500	2.84908800
C	7.04922500	-4.67579200	2.62010100
O	8.94512400	-3.31353100	3.45147200
P	8.37663900	-2.94489100	4.95143000
O	8.86076500	-1.56610700	5.35593400
C	9.55851300	-5.75544000	0.76603100
O	8.42381600	-6.42464100	0.20730900
O	1.10978500	-3.50600700	-0.45640000
O	6.69519700	-2.85798300	4.77069200
C	6.15475400	-1.62779100	4.28267400
C	6.03719100	-0.58397800	5.40179600
O	4.71009300	0.00190200	5.24822900
C	4.10990700	0.25818200	6.53427200
C	5.09005900	-0.22908600	7.61075800
C	6.09988400	-1.11855600	6.86043800
N	2.81006600	-0.47823000	6.56209300
C	1.57298100	0.29654800	6.69222600
N	0.37285000	-0.37466700	6.69292500
C	0.31682300	-1.73666300	6.51370600
C	1.53513100	-2.50339900	6.34958700
C	2.73763600	-1.85469600	6.35605600
O	7.38997300	-0.94237200	7.43575300
O	1.67964800	1.51370200	6.80593700
N	-0.90997200	-2.31910000	6.52091300
O	8.54568400	-4.07769700	5.93905300
O	-3.30359000	-0.78373700	6.94415900
C	-3.36072800	0.42903700	6.84435700
C	-4.46400800	1.33100200	6.66200500
C	-4.21551900	2.70581800	6.36003300
N	-2.99216100	3.33162900	6.32254100
C	-1.94664800	2.50972700	6.66549300
N	-2.08426500	1.12348100	6.86382300
N	-5.46569200	3.27957300	6.07116100
C	-6.42902100	2.20912500	6.24907900
N	-5.84520800	1.07149600	6.61143800
N	-0.70420600	3.06902300	6.84643300
C	-5.59420900	4.49484600	5.25952700
O	-6.36407700	5.47505700	6.01277600
C	-7.19874400	6.23683000	5.08654400
C	-6.97648100	5.64185500	3.66762200

C	-6.36927000	4.26631400	3.95240700
C	-8.63230900	6.06397700	5.61989900
O	-8.78206300	4.76474300	6.19904100
O	-6.02380000	6.56106100	3.07962500
P	-5.48317100	6.21241000	1.56353800
O	-6.59946300	5.81536300	0.62298600
O	-4.50587800	7.26735800	1.08061400
O	-4.60932400	4.77636200	1.76714000
C	-3.25076900	4.91374800	2.19254200
C	-2.32155600	5.18717200	1.00195400
O	-1.21478900	4.24763900	1.13310300
C	-0.85181200	3.69067200	-0.14617800
C	-1.74827200	4.34778800	-1.20527500
C	-2.92486000	4.94504300	-0.41021700
N	-1.03482800	2.21056800	-0.06014700
C	-2.28969400	1.61705300	0.08115000
C	-2.42730100	0.25846600	0.11979600
C	-1.24587700	-0.57712900	0.02884100
N	0.00000000	0.00000000	0.00000000
C	0.16361300	1.36508800	0.00000000
O	-3.33626300	6.16534600	-1.01865100
N	-1.31529300	-1.93048300	-0.07995900
O	1.25335700	1.92557700	0.03201300
H	-8.85924700	6.81887500	6.39652700
H	-9.40305200	6.10251500	4.83042000
H	-6.82570000	7.28285700	5.14899100
H	-7.89251800	5.61198700	3.04102200
H	-7.17929400	3.51674400	4.06448700
H	-5.72197500	3.86059000	3.14643400
H	-4.58337800	4.96073500	5.11591300
H	-7.48912500	2.39071200	6.12588300
H	-1.20621400	0.53119700	6.94601200
H	0.14357900	2.47869400	6.91366400
H	-3.01720600	3.91866300	2.64995300
H	-3.14101400	5.68913800	2.97622800
H	-1.85534700	6.19914800	1.07422100
H	-3.79702700	4.24774400	-0.37954300
H	-2.06595200	3.64753100	-1.99559900
H	-1.20059900	5.15506800	-1.73753400
H	0.24561500	3.89808900	-0.25588000
H	-2.14963200	-2.43594600	0.19571900
H	-0.45074200	-2.50537900	-0.14872100
H	-3.40381900	-0.20507600	0.23363600
H	-3.15695900	2.28826500	0.15497000
H	10.29360000	-5.58364800	-0.04311700
H	9.97114500	-6.47633300	1.49315600
H	9.88986300	-3.62716000	1.34469500
H	8.99846100	-5.40547200	3.43028000
H	6.77455100	-5.72412900	2.38466200
H	6.41793600	-4.39743100	3.48894000
H	6.88166000	-2.64703400	1.68902700

H	5.69031100	-6.16824700	0.16431700
H	1.45093800	-1.10130200	0.00000000
H	2.65290600	0.86083600	0.54947400
H	4.30327500	0.76306400	1.11500600
H	5.13867600	-1.91735000	3.90799700
H	6.73292100	-1.23566300	3.42201100
H	6.75478000	0.25809700	5.24958100
H	5.82961300	-2.19967100	6.92249700
H	4.58730700	-0.74855400	8.44371800
H	5.61602000	0.62898600	8.08204500
H	3.88997400	1.35763100	6.55501200
H	-1.03807800	-3.28169200	6.24520800
H	-1.77835500	-1.75656500	6.63922800
H	1.47877700	-3.57632700	6.18541300
H	3.68621600	-2.38767000	6.20044700
H	-3.61789400	6.85486100	-0.25198500
H	7.87655000	-5.74184300	-0.28103700
H	8.12101700	-0.90384800	6.65486100
H	-7.96826700	4.58040500	6.75480500
H	-0.57126400	4.05019700	6.64291300
C	3.50907300	-3.77543600	3.50170500
C	-0.74633300	2.16045600	3.53843700
H	3.05217300	-6.40027700	3.41035100
H	1.58966500	-7.20440900	2.83694500
H	2.66698600	-6.42061400	1.67610200
H	4.11746900	-4.38894200	2.82066800
H	3.92667400	-2.74962000	3.46148400
H	3.67854800	-4.16162200	4.51642200
H	2.87893500	-1.22696200	3.45799700
H	1.42426700	0.76542000	3.51482200
H	-0.54098100	2.60655400	2.54831200
H	-1.43152000	2.85489600	4.04682200
H	0.20118900	2.17437700	4.09672800
C	-3.71323100	1.65894600	3.33047900
H	-3.29446900	2.64993400	3.58494400
H	-4.17181000	1.74753700	2.33486400
H	-4.53083900	1.45338200	4.03849800
H	-0.39742100	-5.98705400	2.13963000
H	-4.25393000	-0.96345800	3.30405900