Thread-based fluidic platform for urinary creatinine analysis

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Contents

S1. White Balance

The µTAD was prepared by adding 5 µL of acetic/acetate pH 3.8 buffer 0.10, 0.05 and 0.01M, followed by 0.5 µL of the sensing cocktail. Two different creatinine solutions were tested at 1.0×10^{-7} and 5.0×10^{-2} M, with 3 replicates each. 3 min after adding 10µL of the standard solution, the device was digitalized, changing the white balance setting, and the signal variation was then calculated depending on its setting. Six different settings were checked and the results can be seen in Table S1. The best results were obtained when the incandescent setting was selected, which also had better reproducibility in terms of CV.

Table S1. Increase in hue signal and its coefficient of variation for each different white balance

| White Balance	ΔH	CV (%)
Incandescent (2800K)	0.0110	1.0
Sun (5500K)	0.0057	1.0
Cloudy (6500K)	0.0047	1.1
Fluorescent 1 (4000K)	0.0077	1.8
Fluorescent 2 (5000K)	0.0023	2.5
Fluorescent 3 (6000K)	0.0047	1.0

S2. Influence of membrane activation

In previous works, we have demonstrated the suitability of the H colour coordinate for monitoring sensing membranes based on ionophore-chromoionophore chemistry using a bitonal pH indicator instead of a 1-α parameter. This simplifies the calculation and procedure of use, requiring only one measurement per membrane[1–3].

In order to check the use of H for ETH7075 indicator, two sets of sensing membranes were prepared by spin-coating, adding 15 µL of the cocktail on a piece of Mylar sheet, spinning at 190 rpm and letting it dry in a THF atmosphere

To perform the assay, 8 creatinine standard solutions, buffered to pH 3.8 by adding 0.01M acetic/acetate, were prepared (1.0×10^{-7}, 1.0×0^{-5}, 5.0×10^{-5}, 1.0×10^{-4}, 5.0×10^{-4}, 1.0×10^{-3}, 1.0×10^{-2} and 5×10^{-2} M) with 3 replicates each. One set of membranes was used by introducing it directly into the buffered standard solution for 3 min before digitalizing it with a camera. The other set was first introduced into a 0.1 M HCl solution for 3 min to

activate the sensing membrane and then into the standard solution for another 3 min. The second set was measured for both the H coordinate and absorbance.
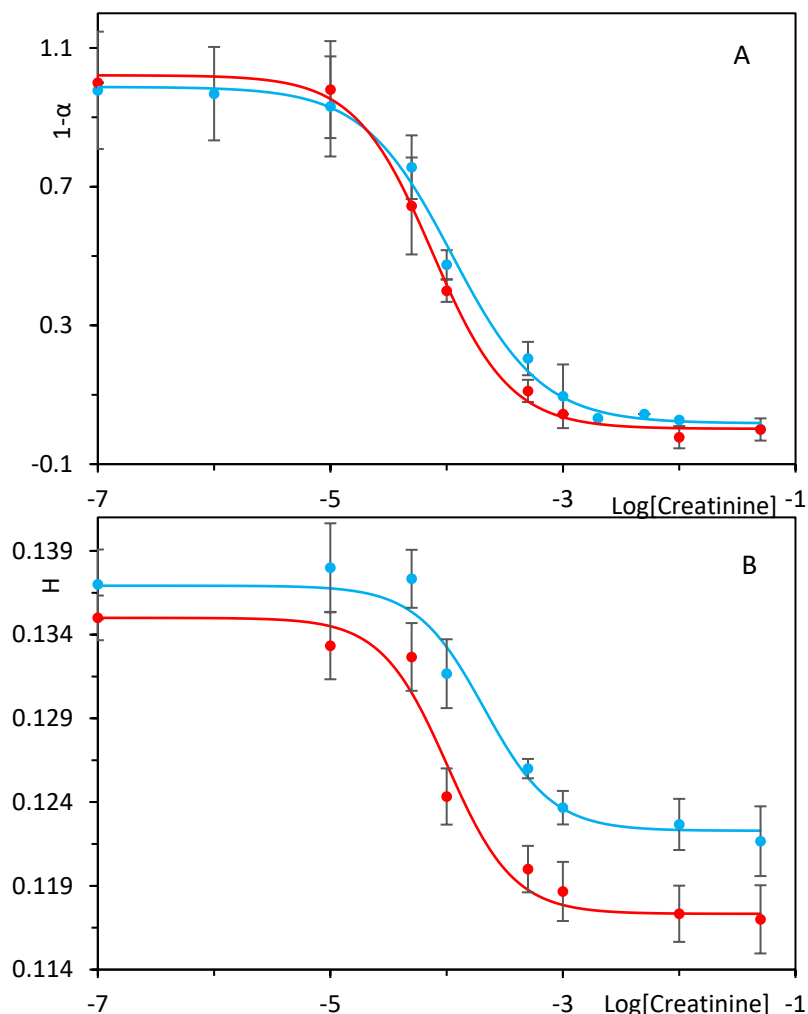
Figure S1. Calibration obtained from activated membrane (blue line) and without activation (red line), using A) 1-α, and B) H as analytical parameters.

S3. Cocktail concentration

The sensing cocktail comprises a solution of 0.88 mg (0.9 wt. %) of ETH7075, 3.2 mg (3.2 wt. %) of calix[4]pyrrole, 1.5 mg (1.5 wt. %) of KFMPB, 63.9 mg (63.0 wt. %) NPOE and 31.9 mg of PVC (31.5 wt. %) 1 mL of freshly distilled THF [4]. From this cocktail, four different dilutions were obtained by adding THF, thus obtaining the sensing cocktail in the 5 different concentrations that were tested. The µTADs were prepared by dropping 0.5 µL of the cocktail on a scoured cotton thread and then letting it dry. Subsequently, three creatinine solutions ($1x10^{-7}$, $1x10^{-4}$ and $5x10^{-2}$ M) buffered to pH 3.8

were tested, adding 10 µL on one end of the µTAD and digitalizing after 3 min, obtaining 3 replicates from each solution.

The H variation from the concentrated to the diluted solution is shown in Table S2 along with the CV of the measurements obtained for each sensing cocktail.

Table S2. Signal variation of µTAD depending on the concentration of sensing cocktail tested on thread

Cocktail:THF	ΔH	CV (%)
1:0	0.015	0.4
1:1	0.014	0.9
1:2	0.004	0.8
1:3	0.001	2.3
1:4	0.003	2.0

S4. Buffering of sample in the µTAD

The µTAD was prepared by adding 5 µL of acetic/acetate pH 3.8 buffer 0.10, 0.05 and 0.01M and then 0.5 µL of the sensing cocktail. Non-buffered $1x10^{-7}$ and $5x10^{-2}$ M creatinine solution were tested (n=3), comparing the results obtained with those obtained using a buffered standard solution. The results are presented in Table S3.

Table S3. H values obtained at two different concentrations when the standard is buffered by the addition of the buffer and those obtained when buffered on the µTAD

Acetic/acetate buffer pH=3.8	Buffer location	$1x10^{-7}$ M (H)	$5x10^{-2}$ M (H)
0.01 M	Solution	0.1399	0.1247
0.10 M	Thread	0.1397	0.1247
0.05 M	Thread	0.1327	0.1250
0.01 M	Thread	0.1323	0.1247

S5. Response time

The reaction time for the μTAD was studied using two different creatinine solutions, 1×10^{-7} and 5×10^{-2} M, with 3 replicates each, taking pictures at different times (10, 15, 20, 30, 60, 120, 180 and 240 s).
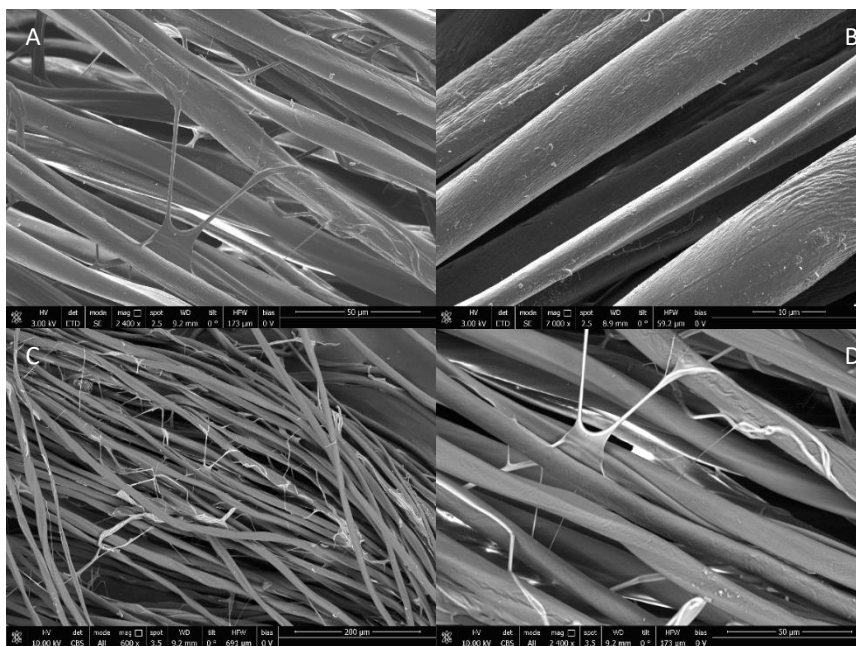
Figure S2. μTAD images obtained by FEG-ESEM using CBS and ETD. A, C and D show the PVC membrane containing the reagents located in the hollow space between yarns like a 'sensing web'

S6. Calibration

To calibrate the μTAD, 11 creatinine standard solutions were tested (1.0×10^{-7}, 1.0×10^{-6}, 1.0×10^{-5}, 5.0×10^{-5}, 1.0×10^{-4}, 5.0×10^{-4}, 1.0×10^{-3}, 5.0×10^{-3}, 1.0×10^{-2}, 5.0×10^{-2} and 9.0×10^{-2} M) with 5 different replicates each. The photographs were taken in the same controlled situation described in the 'Measurement setup' section in the manuscript at 30 s, counting from the moment of the sample addition. The photographs were acquired and analysed with a smartphone running an in-house app[5].
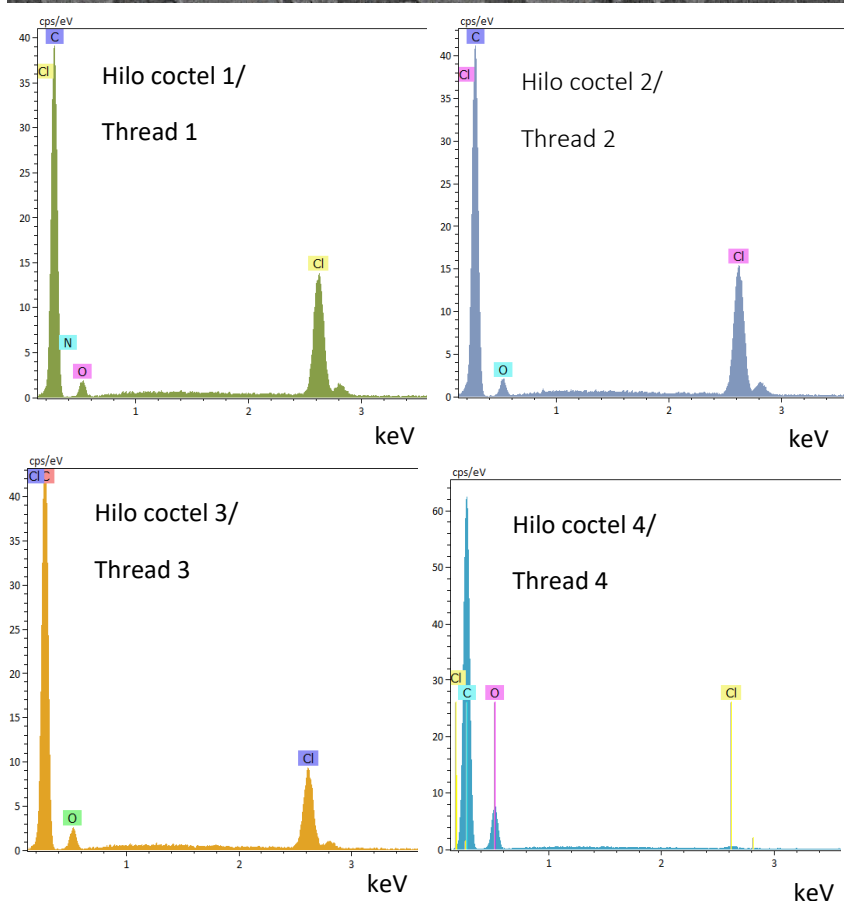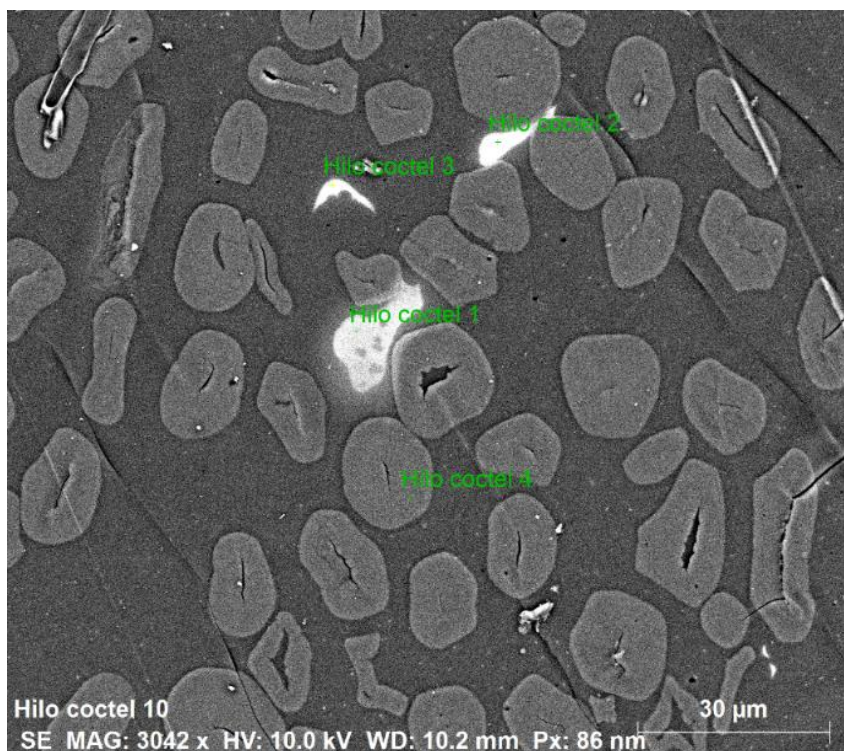
Figure S3. EDX analysis cotton thread with and without sensing cocktail. The presence of Cl comes from the PVC used to obtain the membrane on the thread. Thread without sensing cocktail contains a very low quantity of Cl.

S7. Selectivity study and maximum tolerable error

To calculate the selectivity coefficients for the sensing membrane studied, the separate solutions method[6] was used. The response curves (n=3) for creatinine, Na(I), K(I), $NH_{4(I)}$ (1.0×10^{-6}, 1.0×10^{-5}, 1.0×10^{-4}, 1.0×10^{-3}, 1.0×10^{-2}, 1.0×10^{-1} and 1 M) uric acid (3.0×10^{-5}, 1.5×10^{-4} and 3.0×10^{-4} M) and urea (1.0×10^{-6}, 1.0×10^{-4}, 1.0×10^{-3}, 1.0×10^{-2}, 1.0×10^{-1}, 1 and 2 M) were obtained. The results obtained are shown in Figure S3. The corresponding exchange constant for each equilibrium was calculated assuming a stoichiometric index of p = 1. Finally, the selectivity coefficient was calculated using Equation S1, where a_{H^+} is the protonic activity in the sample, and C_R, C_I and C_L are the molal concentrations of the lipophilic salt, liphophilic pH indicator and ionophore, respectively.

$$k_{IJ}^{opt} = \frac{v}{z} \frac{K_e^{JL_q}}{K_e^{IL_p}} \left(\frac{a_{H^+} \alpha}{1-\alpha} \right)^{z-v} \frac{C_L - \frac{1}{v} C_R - (1-\alpha)C_C}{C_L - \frac{1}{z} C_R - (1-\alpha)C_C} \qquad \text{Equation S1}$$

The selectivity coefficient calculated was compared with the selectivity factor $K_{ij}^{opt}{}_{max}$, calculated using equation S2.

$$K_{ij,max}^{opt} = \frac{a_{i,min}}{(a_{j,max})} \cdot \frac{P_{ij}}{100} \qquad \text{Equation S2}$$

This value depends on the minimum concentration of analyte in the sample ($a_{i,min}$, 5 mM creatinine), the highest concentration expected of the interfering specie ($a_{j,max}$, 100 mM K(I), 200 mM Na(I), 20 mM NH_4(I), 3.5 mM uric acid and 250 mM urea) and the highest tolerable error in the activity a_i due to the interference of a_j (P_{ij}, 1, 10 and 100%).
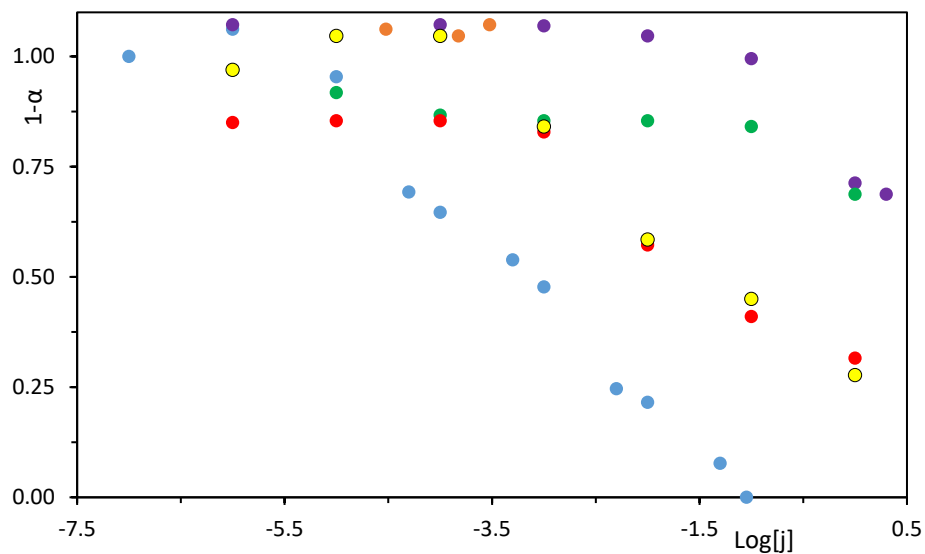
Figure S4. Response of the µTAD in the presence of different species (j) (n=3). Creatinine (blue dots), Na(I) (green dots), K(I) (red dots), NH4(I) (yellow dots), uric acid (orange dots,) and urea (purple dots)

Artificial urine tested was prepared as described by Zhang[7]; the composition is shown in Table S4.

Table S4. Composition of the artificial urine tested

Species	Concentration (mM)
Creatinine	1.0
Urea	100
NaCl	440
Na_2SO_4	15
KCl	40
$MgCl_2$	4.0
NaH_2PO_4	20
$CaCl_2$	4.0
$Na_3C_6H_5O_7$	2.7
pH	6.0

S8. Real sample analysis

The pre-treatment of the samples was studied using a freshly obtained urine sample that was diluted in water (1:0, 1:50 and 1:100) using a 0.22 µm filter when filtered. A kinetic study of the µTAD was performed, obtaining a picture at 30, 45, 60, 120, 180, 240, 300 and 360 s (See Figure S5). The µTADs used were prepared by adding 5µL of acetic/acetate pH 3.8, 0.10M buffer, and 0.5µL of the sensing cocktail. The creatinine concentration obtained using different dilutions was compared to the value obtained using a reference method (Jaffé) [8](See Table S5).
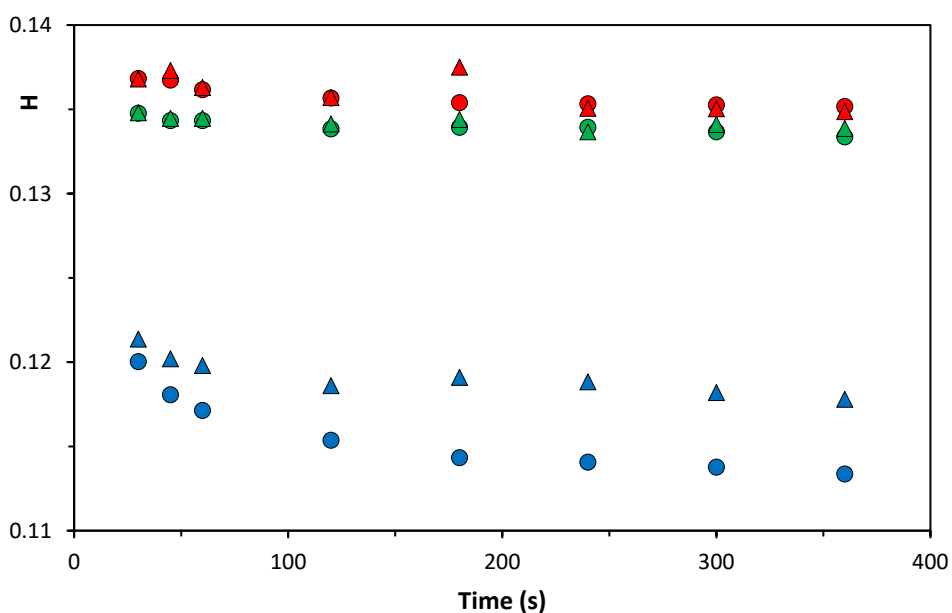
Figure S5. Kinetic study of the µTAD depending on the sample treatment performed (▲) Filtered sample; non-filtered samples (●); 1:0 dilution (blue data); 1:50 dilution (green data); 1:100 dilution (red data) (n=3)

Table S5. Creatinine concentration predicted depending on the sample dilution

Urine dilution	Creatinine concentration, mM			Error (%)
	Sensor (H value)	Sensor [C]	Reference (Jaffé)	
1:0	0.073±0.059	Out of range		Out of range
1:50	0.130±0.001	35.7	17.5	104%
1:100	0.132±0.001	18.1		4%

S9. References

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[8]   J.M. Pizzolante, Stabilized alkaline picrate reagent for Jaffe creatinine determination, 1989.

S10. XYZ coordinates (Å) and Total Energy (Hartree) for all the complexes 1–18 studied, optimized at the DFT theoretical level (PBEh-3c)
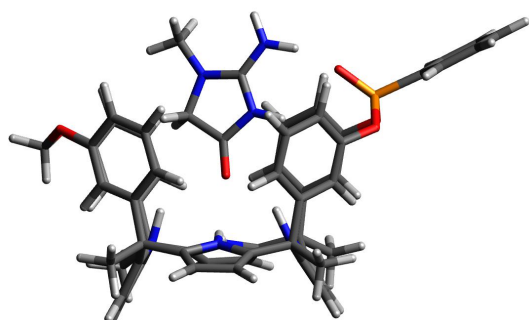
Complex **1** *(upper rim)*, $E_{tot}(Hartree)$**: -3450.175983144803**

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C	-2.16928617320751	4.04733362491895	-2.83178332238625
C	-1.77549564968771	4.57356435320160	-1.57679188998432
C	-0.89459242739592	3.68724580314242	-1.01247871823608
N	-0.75792653041125	2.64751549793462	-1.88878605234511
C	-1.67239610013128	1.80932359938340	-4.08078138606662
C	-0.26933208834336	3.68037937122862	0.35786244248640
C	1.19985704632686	3.33718654634567	0.30626258150742
C	2.30761181245182	4.14216894736189	0.34306617471742
C	3.45047264629834	3.30357029300075	0.34869265127289
C	3.01567762209768	2.00505571442413	0.31345215454755
N	1.64787230806112	2.04407063985139	0.25663026819255
C	3.77646683379120	0.70511725338826	0.40266828056176
C	3.91135544994399	0.03429303917773	-0.94025748831501
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C	1.28031067322508	-2.46026227923240	-3.37973416258701
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C	1.99316222505361	-1.93862787075781	3.35873791863115
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C     0.13819944702507       -2.77351691425212       -4.12018291208464
O     1.54675614281915       -0.00008277150907        4.71495042429009
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C    -2.54379099272417       -3.33750845055300       -5.23694192310801
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N   -0.85972496497764     -1.37450566071803      1.38346571862945
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C   -1.87596240335832     -1.90391804705751     -0.60689275944100
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C   -3.63190687042360     -3.44926896471255      0.42151319128493
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H   -2.95247520112975     -3.22849535929420      3.03835830106898
H   -4.00025946760405     -3.41811764644536     -0.59992430271655
H   -4.45168474461897     -3.15235755517090      1.07621707227823
H   -3.33684868916081     -4.47486607861542      0.64584437104328
H   -1.42812504884947     -2.63913450441367     -1.28332916159382
H   -2.56723534727481     -1.27511619336084     -1.17304834532669
H   -0.23608259994089     -1.00642510058740      2.09419718466970
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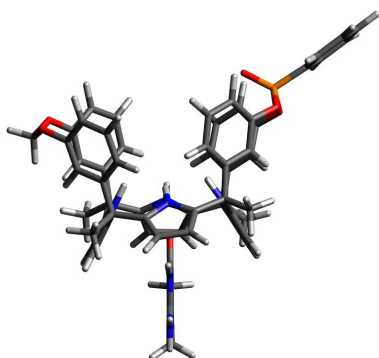
Complex **1** *(lower rim),* $E_{tot}(Hartree)$**: -3450.142159799865**

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C	-5.854290731	-3.052899329	-9.130463782
C	-4.948070994	-2.908772579	-8.107509626
N	-4.214324862	-1.793621672	-8.379161468
C	-4.093913983	0.117951993	-10.024971326
C	-4.700862313	-3.769024527	-6.892362351
C	-5.067825294	-3.018812289	-5.631183330
C	-6.194323470	-3.086678458	-4.846285581
C	-6.017295853	-2.187959552	-3.762919837
C	-4.786051753	-1.598253466	-3.913615034
N	-4.236106285	-2.111189829	-5.049373216
C	-4.067615510	-0.578531992	-3.055351978
C	-4.403073708	0.810443730	-3.544279360
C	-5.210527566	1.771098402	-2.983636765
C	-5.253930864	2.870663472	-3.884541237
C	-4.457584554	2.551552272	-4.965742493
N	-3.962465318	1.305366569	-4.735917772
C	-4.128894825	3.353033805	-6.204089249
C	-4.680732128	2.663701248	-7.429426714
C	-5.794428594	2.917018226	-8.194233317
C	-5.781033606	2.005069841	-9.283580893
C	-4.658390100	1.222454729	-9.153328071
N	-4.024162373	1.630431446	-8.022455409
C	-2.614135886	3.565143966	-6.339185747
C	-2.560205320	0.196871838	-10.017427977
C	-3.245276470	-4.243775978	-6.847894032
C	-2.560870931	-0.860547440	-3.042720580
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C	-5.571918196	-5.030755015	-6.985591312
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C	-2.133366531	-2.177661771	-2.873634046
C	-0.785925674	-2.472616230	-2.778165717
C	0.175600594	-1.476644136	-2.852211357
C	-0.247864103	-0.169384236	-3.015741046
C	-1.599215831	0.140734261	-3.106012473
C	-2.505034108	-4.402731058	-8.015946031
C	-1.216183470	-4.914220248	-7.973805423
C	-0.633385804	-5.279207892	-6.770867309
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C      -0.356095274     -0.763083559     -9.964472202
C      -1.738760841     -0.918039926     -9.937681225
C      -1.785344417      3.571280719     -5.223454780
C      -0.432582944      3.854693294     -5.363339968
C       0.113258932      4.132724361     -6.603138905
C      -0.716290152      4.160186366     -7.720919952
C      -2.069813324      3.872200480     -7.587163571
O      -0.422870582     -3.785624023     -2.548264844
O      -0.867190560     -5.537437714     -4.392961886
O      -0.134465150      4.546914306     -8.884185192
O       0.054438854      2.788007183    -10.356905083
C      -0.531834820      4.028579805    -10.114294251
P       0.304807386     -4.708292101     -3.654357447
C       1.094648425     -5.946524215     -2.656993195
O       1.113884890     -3.921144651     -4.617962423
C       1.259898585     -7.236617311     -3.158267179
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C       2.482689506     -7.838188272     -1.181010786
C       2.321763674     -6.554047821     -0.682032643
C       1.631038859     -5.605304529     -1.416716506
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H      -6.558877714     -3.860052416     -9.251810118
H      -3.504314239     -1.401832100     -7.774816749
H      -7.031184345     -3.751790677     -4.987004115
H      -6.700575420     -2.045131362     -2.940923198
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H      -5.731445749      3.821972725     -3.710005468
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H      -5.321670230     -5.603345717     -7.877336094
H      -5.412888301     -5.667534090     -6.116722926
H      -6.632522988     -4.781600311     -7.030806164
H      -4.211252397      1.288852674    -11.854636137
H      -4.155332576     -0.455147826    -12.114282500
H      -5.643929637      0.309993748    -11.557515034
H      -5.854549639      4.669763682     -5.960670251
H      -4.572652013      5.332528853     -6.971128198
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H     -2.156168395    -1.911940148    -9.862276526
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H     -2.726818588     3.915044865    -8.445709039
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H     -0.126074634     4.712772873   -10.856173330
H      0.843506013    -7.515821016    -4.116560056
H      2.076815604    -9.180726860    -2.803428237
H      3.022378257    -8.577101574    -0.604143805
H      2.732676386    -6.290141297     0.282597420
H      1.505294388    -4.609148617    -1.014771816
N     -9.044373273     0.218221910    -6.681200906
C     -8.628073506     1.030329127    -5.723121133
N     -7.303748910     0.967191209    -5.566723779
C     -6.748235851     0.057145329    -6.478835503
C     -7.916157424    -0.491946843    -7.262399292
O     -5.599674120    -0.199267370    -6.581000993
N     -9.415858609     1.808139222    -4.999867414
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H    -10.409519676     1.839995529    -5.147216727
H    -10.450408061    -0.678979229    -7.897407162
H    -10.883110403     0.947613348    -7.405753641
H    -11.011399699    -0.408295948    -6.252701711
H     -7.989921508    -1.573230088    -7.123837891
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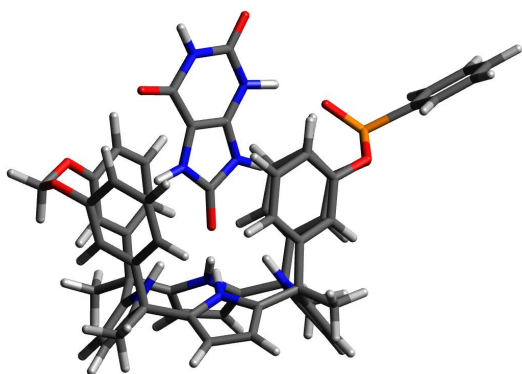
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O	5.08939937670433	0.12322991588100	3.73067215587947
N	3.18405330897304	-0.19400975435945	2.53263716923482
C	2.55596575050588	0.01113420273504	1.35279539333839
N	1.28351524473623	-0.33517083642975	1.01473522654984
C	1.02870432536936	0.05886224163437	-0.28102073842045
O	-0.04087084834045	-0.09211857211790	-0.88311595191882
N	2.16082705385122	0.63576821789546	-0.71952531555416
C	3.12589695140734	0.60379152398854	0.27591187460684
C	4.48352567840591	1.05238044929578	0.30748104501988
O	5.10617103823903	1.59853297088038	-0.57261375078317
H	6.02213629184674	1.06168224683884	1.66193499498542
H	2.62756953585583	-0.37021423536806	3.37279078828975
H	0.61494487474348	-0.81800385892958	1.59798349498199
H	2.29615170529744	1.00482870140801	-1.64980052125942
C	-1.43252807225579	-3.22157055853416	-2.79688434609571
C	-2.31586648831629	-4.26982657452595	-2.84218939048882
C	-3.14184451101577	-4.18405815518335	-1.69493148092347
C	-2.74120476498635	-3.08523504954281	-0.97694562134716
N	-1.71218519592305	-2.51168311544843	-1.66616444497539
C	-0.34750754604724	-2.81339998276572	-3.76279458205380
C	-3.19962694662522	-2.58013011452798	0.36850590643066
C	-3.74822665527155	-1.17575326724804	0.29436507687881
C	-5.02310025449111	-0.69973764451674	0.46839064679768
C	-4.96546740235783	0.71585724881664	0.41585547206588
C	-3.65636080127877	1.06799929637229	0.21217618090225
N	-2.93833913105855	-0.08860467987416	0.12942011454847
C	-2.99062327864766	2.42004184162457	0.11510756231112
C	-2.71115064270773	2.76795400845822	-1.32641666042693
C	-3.26805492036634	3.73507168659163	-2.12488176762548
C	-2.67191212017498	3.62947096673290	-3.40478344764415
C	-1.76486463749468	2.60153052502494	-3.35805163347660
N	-1.81233865067794	2.08577976753274	-2.09503652360322
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C	-0.96208695982047	0.67854970858939	-4.74260772623430
C	-1.36566526989109	0.07911684558012	-5.90906420316764
C	-1.22978643923893	-1.32313024360004	-5.74166737390229
C	-0.74728843852976	-1.54293946156117	-4.47705423268360
N	-0.61175430512914	-0.32227777227003	-3.88425794482828
C	0.66651674218666	2.37381877281847	-3.89513853708478
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C    -4.29597234316678    -3.51480994055446     0.89733464905644
C    -0.15860508739650    -3.93379218386438    -4.79378671822203
C    -0.94595960974650     2.97584127460414    -5.66195028085812
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C    -0.02243623838563    -3.64034614124311     2.22790174824815
C    -0.04721450521649    -2.82431113820256     3.34876223611192
C    -1.09574081868014    -1.92583157705931     3.48207414356179
C    -2.08525068741442    -1.82454325528581     2.51906801995065
C     1.97180547936121    -1.82094236758718    -3.68062407140022
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C     3.49556694083906    -2.19451466103890    -1.86093913602040
C     2.54666034231866    -2.99487150411351    -1.25624958030887
C     1.30431724469303    -3.20744200826284    -1.84355995599996
C     0.95119353432964     3.39178979608385    -2.99016779296177
C     2.26019289465363     3.63643178824561    -2.60035147021456
C     3.30600853875343     2.87650227553737    -3.09699694993451
C     3.03360112282235     1.88290235018363    -4.03075381528068
C     1.72277599009356     1.63119061913828    -4.42165295354650
O    -0.85420058194246     1.40985747655586     4.39013689924832
O    -1.21057648534895    -1.13660371514372     4.61084573795102
O     4.11224652533867     1.24701442381041    -4.56843331517909
O     4.20393906729940    -0.84114940266040    -3.61013544680123
C     4.08548074934614    -0.12321278653222    -4.80232569533741
P    -0.17927364012378     0.06081868840773     4.94175136453789
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C    -0.52274394477099    -0.77249953933261     8.87588407563024
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C    -0.46251051183748     1.50730211298013     7.28822655295801
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H    -3.93711382319948    -4.86428224331319    -1.43779546552239
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H    -4.02735924009638     4.44343488299355    -1.83778550493613
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H    -1.21157704210148     1.35369364481490    -1.74624394986454
H    -1.71640496982576     0.58155600039995    -6.79549445467787
H    -1.46117890130818    -2.07679943320404    -6.47638572899651
H    -0.18732302931893    -0.18709948133541    -2.97867823963320
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H     0.11416101484002        -4.86243142754488        -4.29431432103569
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H    -1.95220364878929         2.86795069969358        -6.06657529728608
H    -0.23107541515288         2.66931224151885        -6.42424895415588
H    -0.77298944208954         4.02914561719059        -5.44584593806188
H    -2.71354772332005         1.40658151889172         2.60707402025151
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H     1.48965348840099         3.49430401424181         1.11416487441181
H    -0.44759998491070         3.46502441856716        -0.38573317501838
H    -0.98712036286292        -4.21439864227884         0.40456147209135
H     0.77643401592279        -4.36154020757883         2.11616487128504
H     0.72172097930528        -2.90009659577145         4.10496953290734
H    -2.89669787793616        -1.12258577038060         2.66801013576057
H     1.72181961536061        -1.38544484988273        -4.63780245904671
H     4.45932056220088        -2.01883326192266        -1.40128791491385
H     2.77525315121402        -3.45877475837849        -0.30511963482542
H     0.57969962741185        -3.84055724593547        -1.35113394950822
H     0.14926841469231         4.00654617563194        -2.60177690803061
H     2.46942941107539         4.42627493727171        -1.89048345794045
H     4.32479888752165         3.04505154036302        -2.77913513861447
H     1.50912986874704         0.87691575739494        -5.16985853530937
H     3.21413950188120        -0.42992274244707        -5.38751909056699
H     4.98085394415712        -0.32408231936484        -5.38942399974376
H    -0.36394642965374        -1.88077244232117         7.05836473774333
H    -0.55009724504650        -1.65996735167801         9.49317237457377
H    -0.69114905329113         0.57801912627254        10.53190465491653
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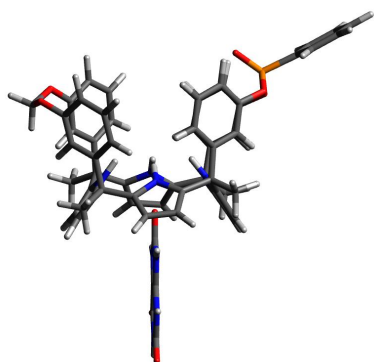
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C         3.021978178      8.160282519      1.341343053
C         2.778262683      8.017787624      2.698708844
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H        -7.101570476      0.531732545      0.684702663
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H	3.994277773	8.487584358	0.998290684
H	3.558681901	8.231015451	3.416312131
H	1.360003890	7.481928771	4.203262105
N	-7.734256682	-4.127904844	5.338239919
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O	-7.265491075	-5.027189394	7.379259683
N	-6.930009284	-2.805133342	7.059630998
C	-6.992392862	-1.746819519	6.207561960
N	-6.661671392	-0.455806929	6.444071296
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O	-6.679111313	1.485798125	5.171197105
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C	-7.420525306	-1.854560756	4.923939015
C	-7.837366793	-3.101684396	4.378945547
O	-8.236545465	-3.328271750	3.259775460
H	-8.012642642	-5.046809983	5.023950465
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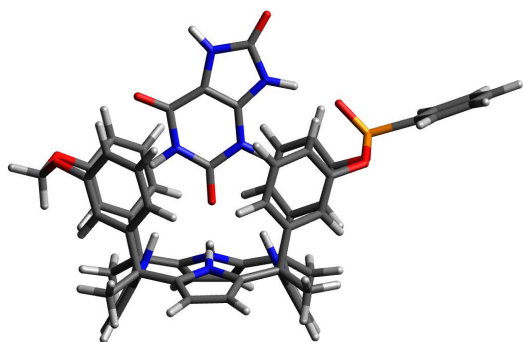
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N	-1.47501712814892	0.22690756048430	1.05421846727608
C	-2.73597389773952	0.34964713822782	1.55136104839389
N	-3.11711717250355	0.43007229390205	2.84270608289649
C	-4.51414862561522	0.54603736390907	2.91625406910928
O	-5.18088552401842	0.63282251266817	3.91471549987946
N	-4.92269114338665	0.53654548605147	1.60542268783346
C	-3.83398703181573	0.41215641640098	0.75802414141504
C	-3.74051061803820	0.34737491389441	-0.65599454627896
O	-4.64005289247825	0.40544638144598	-1.46172537307703
H	-2.25263835410807	0.11911549559729	-2.06026437682578
H	-0.67174344958795	0.20416309099856	1.66659292747596
H	-2.49274275846299	0.37956601623765	3.65540681780348
H	-5.88359199660083	0.60072162058640	1.32047671011038
C	1.96457753047405	2.81543557815453	-2.96227683242374
C	2.82700119114855	3.87548740463226	-2.84624896775564
C	3.44625209249863	3.78680290825097	-1.57593241591578
C	2.94724776203174	2.67394323312417	-0.94730972265573
N	2.05192690118977	2.10025914610779	-1.80326658384887
C	1.04357249005397	2.42247265649096	-4.08883138911864
C	3.24071686940878	2.12024433783648	0.42291492032131
C	3.65041244473866	0.66792391680169	0.35702289239261
C	4.88927190966586	0.08214428020849	0.39907708005533
C	4.70111517361332	-1.32252425639593	0.40999544426500
C	3.35157335189569	-1.56137805207164	0.37424027116797
N	2.73299541136957	-0.34388572797393	0.32016344283445
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C	2.16280307636126	-3.31032693157035	-0.93601050750209
C	2.33713718822841	-4.52218179504306	-1.55485978942763
C	1.75045378380322	-4.43411760868723	-2.84000158986056
C	1.23197680345475	-3.17097338795463	-2.97517367746835
N	1.49260382765811	-2.50706430829661	-1.81219507568938
C	0.45385118596176	-2.55463499465212	-4.10959213727211
C	1.05209871408419	-1.23404540967218	-4.53356303452162
C	1.85402393280767	-0.90584149204315	-5.59591759856647
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O     0.78257317973371     -1.40087226039702      4.74683440761344
O     1.18195144123365      1.14967756080552      4.74348236416202
O    -4.03290077830584     -0.65860148483581     -5.03416504598754
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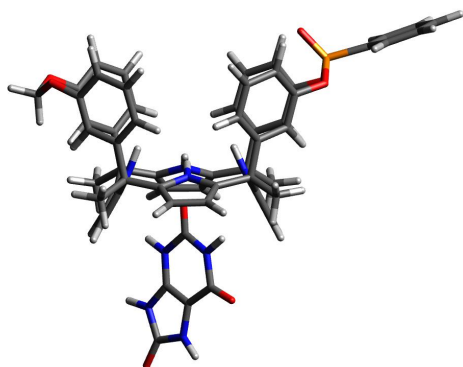
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H	5.359512016	-4.929303542	-4.803871465
H	8.259506067	-4.258190566	-1.951099332
C	1.763948987	-1.277745857	-5.354710327
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C	3.303790399	0.142737089	-6.174455081
C	2.925258849	0.599144880	-4.937105388
N	1.992446872	-0.274729963	-4.457960736
C	0.771750592	-2.382946779	-5.098061580
C	3.368082958	1.822470404	-4.177103002
C	3.851843469	1.467954346	-2.790841497
C	5.120746974	1.310668469	-2.296044408
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C	3.682062503	1.110428708	-0.576628690
N	2.993340615	1.321295781	-1.738113847
C	2.985157278	1.003991320	0.759013799
C	2.484107980	-0.396192878	0.999363192
C	2.671907298	-1.232462585	2.070504369
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C	1.372368541	-2.301144172	0.575996470
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C	0.947947225	-3.471292874	-1.583457644
C	1.634202071	-4.516031889	-2.146461875
C	1.718931000	-4.274076382	-3.541830828
C	1.082416439	-3.087747244	-3.797690008
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C      0.856773941      -3.394214115      -6.251195733
C      0.447712894      -4.591175695       0.569597381
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C      1.152326603       4.328868387       0.549558782
C     -0.104014017       4.042560518       1.064176490
C     -0.368219292       2.739246774       1.451756555
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C      1.126274641       2.850940622      -4.887074542
C      0.191314202       3.876276745      -4.827198998
C      0.360475920       4.951109625      -3.969244807
C      1.488072619       4.969047875      -3.160564406
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C     -1.436640722      -1.776501067       0.709207816
C     -2.776344687      -1.406658722       0.714966587
C     -3.674697496      -1.963507070      -0.173821987
C     -3.229843486      -2.921800648      -1.080709314
C     -1.894612775      -3.303030872      -1.082530442
O      1.499808950       5.624131674       0.203985453
O      1.752647356       6.044844602      -2.330554346
O     -4.185698307      -3.473290930      -1.874382863
O     -4.034395761      -3.075735940      -4.144237270
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C      1.332226614       8.092505892      -0.715957264
O     -0.586760928       6.122488014      -1.243210834
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H      4.035419477       0.594724199      -6.823499502
H      1.507089344      -0.176252176      -3.581698944
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H      5.832354599       0.927805593      -0.217739073
H      1.993793210       1.449880069      -1.795644724
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H      1.922688995      -3.294566032       2.447595324
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H      0.039481219      -1.808338317      -2.492926493
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H      0.165726457     -4.219728318     -6.089151619
H      0.593894621     -2.914698908     -7.193239228
H      1.861918021     -3.805494903     -6.343607510
H      1.451314449     -5.007109168      0.656305503
H     -0.176347364     -5.310208541      0.041975348
H      0.039642130     -4.466414366      1.571387618
H      3.091509861      3.611116699      0.023477061
H     -0.849192589      4.817857508      1.173341319
H     -1.343293000      2.494212307      1.851952156
H      0.371333648      0.742140211      1.667052178
H      0.983497490      2.035972387     -5.583444827
H     -0.681326608      3.843804466     -5.466073644
H     -0.359653409      5.756950373     -3.937026628
H      3.289727797      3.998248830     -2.557880350
H     -1.392666560     -3.686867954     -4.231713426
H     -4.376711825     -0.710660831     -4.999520827
H     -2.623914164      0.765764484     -5.925165393
H     -0.271296004      0.041820114     -5.973048888
H     -0.751911442     -1.337581831      1.422073145
H     -3.124422224     -0.664441333      1.421712137
H     -4.712557492     -1.662668002     -0.187157419
H     -1.538717224     -4.075703723     -1.752469841
H     -2.920572336     -4.506854484     -3.145242754
H     -4.664470603     -4.761715367     -3.306729970
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H      2.009820792     10.973552739     -2.356892039
H      2.122940273     11.803747603     -0.032936167
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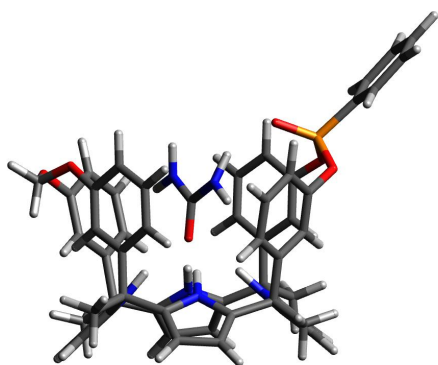
Complex **3** *(upper rim)*, $E_{tot}(Hartree)$**: -3279.271963056833**

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C	-0.63982303492560	3.48521182376169	-1.59073275410949
N	-0.93142208383177	2.25090579506864	-2.09492552584275
C	-1.96405780572277	1.15986691047320	-4.12286400835105
C	-0.07500301163669	3.69024943725407	-0.20495752056192
C	1.37617460046617	3.27855949339254	-0.15131530498323
C	2.50990653261998	4.02841583338008	0.02776111528343
C	3.60803116128989	3.13515204128202	0.07810606197571
C	3.11821590918804	1.86197024842154	-0.07229899697608
N	1.76402043179341	1.97205313269866	-0.21814565848723
C	3.83355654494738	0.53448446679777	0.00040059783484
C	3.71220001103597	-0.26052846125818	-1.27888726135912
C	4.68388169171700	-0.70261476207216	-2.14228170631676
C	4.05915896186201	-1.53501090789554	-3.10347261469466
C	2.72132671633854	-1.58130242924006	-2.80244692235401
N	2.53111922670731	-0.79809456113382	-1.70237077406027
C	1.58214838275632	-2.31637241076888	-3.47002648224263
C	0.72096659931484	-1.35101024162887	-4.24941606360314
C	0.54001092836134	-1.19039643600479	-5.59556169291620
C	-0.45800519889329	-0.19949451387314	-5.77988938024250
C	-0.86027316274286	0.21636343137008	-4.53449851915603
N	-0.12131655916280	-0.48066675728531	-3.62431269549597
C	0.73343784146915	-3.06623377145321	-2.43019478922834
C	-3.02165252119404	0.42672654302264	-3.27927947499840
C	-0.88108678708592	2.92822011019334	0.85620186076398
C	3.31539921290417	-0.30235398028567	1.18233645023062
C	5.32133718103362	0.79848311144813	0.27335384088712
C	-0.18417106680458	5.17957303023423	0.15308507496937
C	-2.67869791582920	1.65841389018703	-5.38654030923492
C	2.15783261403595	-3.36321370347344	-4.43056100492888
C	2.72100078336705	0.29794485611325	2.28933356472478
C	2.29195041981963	-0.47339034727562	3.35799337377003
C	2.46265386919056	-1.84675493461577	3.36927956544548
C	3.08222416906398	-2.44328176109543	2.28085930159232
C	3.49275605621660	-1.68571855236953	1.19470655149073
C	-2.23763357138582	2.66525220087332	0.69440753029755
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C   -3.85922217930792     1.14453152425478    -2.42941009307024
C    1.30560907554145    -3.59750740366022    -1.28099291522103
C    0.51334677597132    -4.26657774086672    -0.35983761674433
C   -0.84560924798398    -4.41641073577608    -0.56140645032068
C   -1.42285291160829    -3.90646314771891    -1.71940420106411
C   -0.62811717776661    -3.25710847061637    -2.65342190629086
O    1.70700190572219     0.15385783719003     4.44078655869984
O   -0.37736175367142     1.63658624740641     4.23858281130016
O   -2.76854542183224    -4.07966457540326    -1.82497677044138
O   -4.49007309247251    -2.92565774849623    -2.80629003442504
C   -3.47995323469937    -3.86108042169958    -3.00648493865090
P    0.11008333310384     0.17114260280186     4.69598557453283
C    0.02772537961579     0.30679922691599     6.47500148898354
O   -0.62067180175685    -0.95231575144414     4.06837689871266
C   -0.99871921762625     1.03464100973752     7.07206681196363
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C   -0.24093563764948     0.32946206151653     9.23981090201919
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H    2.55967820890211     5.10141758054791     0.11276652429572
H    4.64109550513509     3.40847757883653     0.21503660666151
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H   -3.09676891839683     0.82021406610466    -5.94161707330071
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H   -1.98971846697555     2.19380384768908    -6.03927660779260
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H    -1.46517379485945     -4.92304982792148       0.16678843713534
H    -1.05019537984139     -2.86933263790381      -3.56780047511973
H    -2.82801945830295     -3.60124348443654      -3.84446198406216
H    -4.00374229883438     -4.78440250837629      -3.25652444513560
H    -1.69361765559814      1.60167158972451       6.46759144408794
H    -1.92681513944715      1.61536592827616       8.90876175054349
H    -0.34577671737769      0.33937982612053      10.31676363747908
H    1.48076566347303      -0.95179132975004       9.26083180862200
H    1.72691591454289      -0.97162604908350       6.82162469659568
C    -0.81997250442460     -0.85776200729872       0.22708798463298
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N    -0.14534394789938     -1.42958555998850       1.22968823207166
H    0.85853542160364      -1.41996779728911       1.18166320664381
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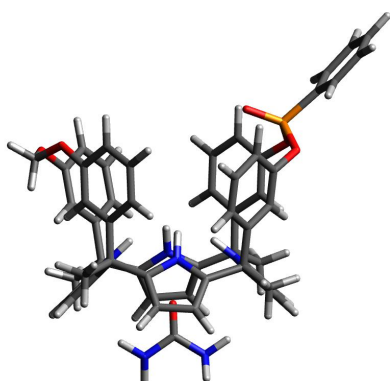
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C	-0.89504003382011	4.10892573845013	-2.53443265448103
C	-0.78052612123909	3.28274956045590	-1.44735680120565
N	-1.26306668698888	2.06167050061564	-1.82885104696326
C	-2.29380492232225	0.88622662273384	-3.81593308751480
C	-0.20052920629844	3.56171605426883	-0.07788870142065
C	1.25547927725133	3.15932112790282	-0.04004145855503
C	2.39857179384547	3.91593477105134	0.01248780191090
C	3.50111062347436	3.02266858572151	0.07349213024816
C	3.00038039983594	1.74426513178026	0.05911404901479
N	1.64547395013402	1.85573433716539	-0.00136874830804
C	3.70182546812471	0.41105638016640	0.13918179779531
C	3.49699566934850	-0.36524678849734	-1.14044497014821
C	4.32435684224652	-0.53600926029312	-2.21894762643816
C	3.65841782981523	-1.37786127017540	-3.14214184675817
C	2.44051509698225	-1.70438995919374	-2.60763933907836
N	2.35364809130858	-1.06443243707795	-1.40355791394583
C	1.31091220394473	-2.51916168327380	-3.19945762087350
C	0.40430840138329	-1.60272599206311	-3.98373028935598
C	0.21338184618325	-1.44350524157607	-5.33270236579471
C	-0.80355110644472	-0.46626020446039	-5.50610843801554
C	-1.20331738278838	-0.05798389914272	-4.25657425285737
N	-0.45865833127636	-0.75830288591277	-3.36122770007152
C	0.50920655230421	-3.25903237697582	-2.11962890738188
C	-3.29034092357464	0.15981851836228	-2.90112359405108
C	-0.97482773629174	2.84591481034778	1.03584703239238
C	3.20177284281073	-0.39567747567336	1.34319326399990
C	5.20342262594565	0.65418808533446	0.34354845892110
C	-0.30543346494063	5.06773635416235	0.20773604144180
C	-3.07993505026420	1.34530921010013	-5.05055400596006
C	1.88717445790632	-3.58194596023365	-4.14494002982063
C	2.63603983404320	0.23103217912839	2.44855824712091
C	2.20989213115603	-0.51330156608409	3.53559574648238
C	2.34193325751955	-1.88998921666890	3.55889680224325
C	2.94017246702217	-2.51242229647592	2.47529084108648
C	3.36689727385745	-1.77831267319070	1.38062565106322
C	-2.33410638729794	2.56850258160845	0.92168454675498
C	-3.01594990143822	1.93414483410619	1.94943762579051
C	-2.37201524270077	1.58603633082664	3.12346906991413
C	-1.03303603941895	1.91233786038720	3.25906241824274
C	-0.33896541449202	2.53121834283447	2.23537244230777

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C    -5.17237552342968      -1.14612139870743      -1.30365431384517
C    -5.01630112031035       0.22541049325809      -1.22339376449336
C    -4.08262870134060       0.87947386786603      -2.01326595369742
C     1.11917521583029      -3.74643391637103      -0.96974893217768
C     0.36341390692399      -4.40834342155860      -0.01114020353323
C    -0.99070773249764      -4.61325133293956      -0.18726849511987
C    -1.60355762837982      -4.16611415642086      -1.35511652660079
C    -0.84980859593543      -3.50525913150147      -2.31450932474303
O     1.68856337398773       0.15499060900861       4.62376579012019
O    -0.37283003991321       1.67928468872835       4.44705818124590
O    -2.93236630836912      -4.42386284793083      -1.44975470741969
O    -4.68504322357497      -3.20071105346541      -2.29496673382698
C    -3.69952252270975      -4.13746295622434      -2.58141087529627
P     0.09430463173358       0.20175733469004       4.92735483383250
C     0.09054665267034       0.39957301950705       6.70795460197758
O    -0.67318605693288      -0.90969981126087       4.34329502531165
C    -0.93180597500744       1.11651437802628       7.32560097925641
C    -1.01460097168343       1.15557299576401       8.70778004280775
C    -0.08162144887812       0.47904672953165       9.47935043031164
C     0.93747126062244      -0.23660606881005       8.86916028153508
C     1.02522100989213      -0.27856451275851       7.48734617309084
H    -1.69135977174875       3.72722114282741      -4.57706699443979
H    -0.58755350924593       5.13998705057973      -2.58571760557723
H    -1.43949328864632       1.30225667644689      -1.19353143435457
H     2.45216894641648       4.99163637237608       0.01974938690918
H     4.54128570800466       3.29577460053404       0.14384294576032
H     1.01812471598812       1.07935895109277      -0.10304898641666
H     5.30841718856960      -0.11530671626062      -2.34224668461633
H     4.03741154009336      -1.69618143655517      -4.09821470218304
H     1.63182957647607      -1.24768176195929      -0.72674732683980
H     0.73898856138449      -1.96718732860275      -6.11349033297263
H    -1.20321135322175      -0.12509398157952      -6.44643867716476
H    -0.50371898328389      -0.64506315922500      -2.36482891692064
H     5.61445022453867       1.24993366551870      -0.47141086088529
H     5.38327295424256       1.18189240968610       1.28036703342476
H     5.74301798205143      -0.29144804817184       0.37595916345253
H    -1.34881812403458       5.37946088460844       0.19522784282458
H     0.11176014268135       5.29671778922796       1.18824462252997
H     0.23520953698076       5.65087008325827      -0.53764257226720
H    -3.54042414293198       0.48969120992407      -5.54346373501386
H    -3.87092216043585       2.03688056960711      -4.76373233370303
H    -2.42820393615123       1.84443318629881      -5.76696006386956
H     2.47444468346609      -3.13059522491597      -4.94438112919410
H     1.08164989950258      -4.15845949953171      -4.59910170723997
H     2.53134173262774      -4.26853771784506      -3.59746860808734
H     2.53723079621316       1.30767405473189       2.48209188458783
H     1.99647001710556      -2.45933026984394       4.41074209442759
H     3.07155331432401      -3.58602508748303       2.48369386926814
H     3.84741141105880      -2.28454831263213       0.55331243884476
H    -2.87299980669662       2.84854734446441       0.02707860363755
H    -4.06336167762207       1.69757744157015       1.82527366412183
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H   -2.90016539081368     -1.75870407395571     -3.74823577490533
H   -5.89028682209165     -1.66587476085078     -0.68422490869299
H   -5.62547409323387      0.79387037826444     -0.53204547418870
H   -3.98229289455384      1.95563860796488     -1.95485335487642
H    2.18123448144446     -3.61178368953433     -0.81418993291252
H    0.84055835886772     -4.76049637844948      0.89380454518343
H   -1.57978011939295     -5.11936414875232      0.56518221282096
H   -1.29878233209124     -3.16249564110368     -3.23426862408099
H   -3.08693037232246     -3.85554295583931     -3.44119124768515
H   -4.24527702351441     -5.04544603120263     -2.83592051163511
H   -1.66198822892788      1.65023881022362      6.73126071923031
H   -1.81276080961318      1.71205374694692      9.17980571094235
H   -0.15047785042293      0.50791591733314     10.55791169147707
H    1.66680689842072     -0.76619237378381      9.46688699785102
H    1.82941796162786     -0.83262710001864      7.02130838092491
H    3.85319310652441      3.05721753598550     -4.00215300237903
N    3.02129882882264      2.96665983748677     -3.44513742957695
H    3.16101674441676      3.11342177783409     -2.45663289603046
C    2.16130323132690      1.93877012664498     -3.74429732614681
N    2.15317177652179      1.57912522219612     -5.07049155177904
H    2.33603642901980      2.29811435612693     -5.74927571724218
H    1.40373118233361      0.95089970661349     -5.31904411910382
O    1.46563344752889      1.39812893003232     -2.91146141798969
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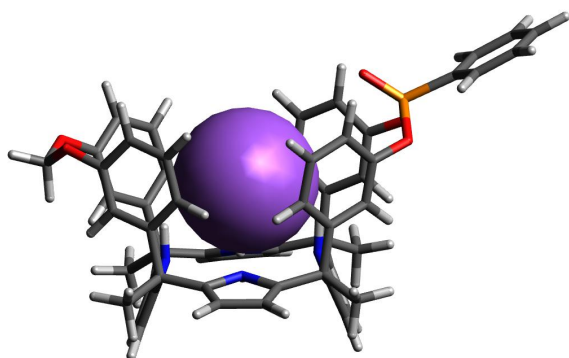
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C	-2.66797621163968	3.56418384320974	-2.72636685558361
C	-2.25332171105239	4.17802471332383	-1.51719464310284
C	-1.26300854304086	3.40411060727386	-0.97745178015401
N	-1.08515991763880	2.33761987596584	-1.81692616879085
C	-2.05458563604603	1.33167361817378	-3.92837852878108
C	-0.56486117789483	3.52229015589666	0.35249334390425
C	0.91461000465361	3.23602222747022	0.21257198855698
C	1.97176487985652	4.05026753439868	-0.08006647308460
C	3.15348982302294	3.25742775635974	-0.05426285293292
C	2.79307887218614	1.97741967757948	0.25984730795812
N	1.41270495850271	1.95514953930354	0.36634569217247
C	3.62296014083578	0.72500137533398	0.42848930025065
C	3.71929299134235	-0.03986431221476	-0.86409589898218
C	4.74640079104217	-0.78574518023217	-1.35136042179213
C	4.27348393315463	-1.47411318510625	-2.50573063776059
C	2.97040313337533	-1.13147059252530	-2.69242860940344
N	2.61009547669191	-0.27596900455183	-1.66192699411261
C	1.97437609578622	-1.64895156395160	-3.69615651762828
C	1.11351075658046	-0.52941939189353	-4.22763808616782
C	1.25286971923692	0.27165233752492	-5.32470853389738
C	0.11430363680710	1.11928407061411	-5.38898224553627
C	-0.69404431107717	0.81866587222473	-4.33007109430612
N	-0.05036779221304	-0.14992624346246	-3.59195198390710
C	1.07915727938351	-2.71520004295360	-3.04177980831848
C	-2.93181126004776	0.18197138348227	-3.38822875215157
C	-1.19274829185811	2.54890065490328	1.36061492345670
C	3.00275218124897	-0.18972853218755	1.49778524602231
C	5.03502300625431	1.09635762819981	0.90960313624238
C	-0.76001284714641	4.94481915176771	0.89879914723968
C	-2.77043012522750	1.89193963673464	-5.16439753633505
C	2.73084193067995	-2.31687166030523	-4.85357686728497
C	2.56232311022022	0.35423305156117	2.70160049481343
C	2.03547698332097	-0.45454995500912	3.69802551480690
C	1.96326073384803	-1.83409138555034	3.54266949528970
C	2.42455723584170	-2.38166102554288	2.35883953193214
C	2.93560582590053	-1.57607306695165	1.34514740932961
C	-2.36010574671053	1.84614513316146	1.08614552373895
C	-2.93281386397101	1.01984492547226	2.04302935607854
C	-2.36670176536835	0.87164895536764	3.29520653160858
C	-1.20061848914207	1.57146956315859	3.56535509309909
C	-0.62242649261586	2.40780973547818	2.62632344856154

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C   -2.88911230456272      -1.08293548272834      -3.98529472986674
C   -3.72438735193410      -2.10382345703824      -3.54498135846383
C   -4.62945762552631      -1.86638026445368      -2.51674925483870
C   -4.69655915866421      -0.60776223342246      -1.95266032505649
C   -3.84764960570097       0.40826273710298      -2.36884135740232
C    1.36998840925273      -3.26634602106362      -1.79448610915133
C    0.55229377187747      -4.26234005987202      -1.26080298990217
C   -0.56740259083638      -4.70045415477449      -1.94141739739614
C   -0.85981076558072      -4.16411654113433      -3.19612192161158
C   -0.02587549406553      -3.19371445074739      -3.74246431967036
O    1.61430593905161       0.15219163061229       4.84353027590087
O   -0.59318423842312       1.47999299212782       4.79665048444873
O   -1.92722304885093      -4.68608398900160      -3.82854029524104
O   -3.78385992631968      -3.34937548944111      -4.09310030939487
C   -2.70717179109497      -3.94362810864580      -4.72967733117680
P    0.05040345212877       0.09113817052956       5.32396483911860
C    0.20578004495424       0.40697625196984       7.06618009769029
O   -0.63594054266083      -1.11516902726324       4.82418239424755
C   -0.77165277956659       1.14359057993610       7.73216163536396
C   -0.68660878401964       1.31460135736810       9.10339497526292
C    0.36639554827625       0.75928698626823       9.81251858627216
C    1.33248352457183       0.01675544256956       9.15216304655956
C    1.25777255036555      -0.16094159169254       7.78170264044359
H   -3.44707144066809       3.90417017036123      -3.38686996393687
H   -2.64531243282685       5.07934472394629      -1.07897191186295
H   -0.31179934047736       1.69877726187049      -1.75665699643843
H    1.92189169817143       5.10821793700302      -0.28356643803368
H    4.15546558418950       3.61133041865899      -0.24035152373298
H    0.94826203849447       1.31743757099582       0.99915142023752
H    5.72754103853225      -0.85837992022808      -0.91333008587210
H    4.83098822320936      -2.16665212631346      -3.11141000974037
H    1.93348788436722       0.45756149536202      -1.82166906557832
H    2.07857227478586       0.26077387899302      -6.01606309435276
H   -0.07194059700640       1.86950794451706      -6.13725422666432
H   -0.58402014519694      -0.79765779864305      -3.03284201837552
H    5.56780162806726       1.68268838455904       0.16116642821136
H    4.98018422908632       1.67763342478137       1.82906706405352
H    5.61210303760202       0.19516580013023       1.11262351961508
H   -1.81930795912775       5.13633119652651       1.06325580564812
H   -0.24301086664051       5.05834106487501       1.85047381269378
H   -0.37521621380039       5.69390231713861       0.20683771263370
H   -2.84195774290587       1.12651033102097      -5.93440362803341
H   -3.78114813569617       2.19938927160563      -4.90394990861525
H   -2.24465512830459       2.75350333584109      -5.57191318041196
H    3.41665190212354      -1.61819923283892      -5.33054346743298
H    2.03527221996364      -2.67966486931706      -5.60721376358849
H    3.30167843864573      -3.16893504717636      -4.48840725239897
H    2.63950872314425       1.41946030086011       2.88638642497982
H    1.57122797684095      -2.46365219358780       4.32938996426897
H    2.42616717282956      -3.45632697996655       2.23417254736426
H    3.35970575212387      -2.04035270348704       0.46473537091626
H   -2.84949108055066       1.96421511980732       0.13182060997866
H   -3.85205642068093       0.50271147680036       1.81056375912228
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H    -2.81652925972625        0.22662758859864        4.03725613452647
H     0.26843608224974        2.95894423363202        2.90877696508343
H    -2.22643104589113       -1.23146119728294       -4.82934888099006
H    -5.28544643023014       -2.66396646463375       -2.19417757642184
H    -5.42475793440027       -0.41450234660466       -1.17597955534571
H    -3.93799693821338        1.39128026484888       -1.92765485695506
H     2.29822577879511       -3.00648549090344       -1.29808384751585
H     0.81589624043633       -4.72530959503213       -0.31642126591278
H    -1.19942707661729       -5.48187925330933       -1.54012420055207
H    -0.20481299793658       -2.81149868582485       -4.74019338720210
H    -2.10852418208599       -3.22710927787051       -5.29480294712295
H    -3.12490970249129       -4.67099742099970       -5.42045611067228
H    -1.59036067865456        1.59302444970874        7.18622953619636
H    -1.44070745898752        1.89238056543950        9.61565188958172
H     0.43027380740017        0.89727926123588       10.88226034010601
H     2.15405610421007       -0.41778065631741        9.70100474894483
H     2.02680128356103       -0.72761495286282        7.27344504287055
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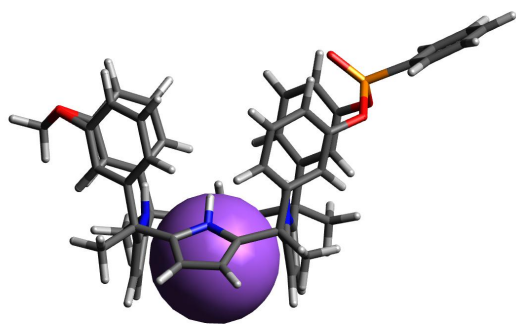
Complex **4** *(lower rim)*, $E_{tot}(Hartree)$**: -3216.354445088705**

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C	−1.89985198303210	4.35945264617695	−1.74517693780418
C	−1.29260583763705	3.40777229560997	−0.98562838230248
N	−1.25010116695726	2.24274610953141	−1.73357405582556
C	−2.04072286326152	1.34361897274468	−3.94788808837849
C	−0.62197054001666	3.49687139235005	0.35823298684129
C	0.83548214845210	3.14557972261325	0.13040504732228
C	1.82549877977370	3.87337757118736	−0.48667389031151
C	3.01317566646886	3.09355773391710	−0.46048837807906
C	2.71982466113340	1.90770445808357	0.17117164545612
N	1.38701846064001	1.94233687850874	0.47597723829711
C	3.60576642338213	0.70774453579530	0.43169555688218
C	3.73181678274434	−0.02646733076975	−0.87478198102154
C	4.81841228184534	−0.35685615576436	−1.62211192968239
C	4.35580205914225	−1.05611812935478	−2.77734827546732
C	2.99971150825160	−1.13486334034047	−2.70232475420719
N	2.60424148129932	−0.45074838455922	−1.56157912920961
C	1.98950435842458	−1.67497186746783	−3.67805603425297
C	1.16170870701842	−0.49200655157968	−4.13823112758496
C	1.45605985143793	0.51893215794018	−5.02155129711263
C	0.31926968309131	1.37024937939535	−5.09795301798245
C	−0.64062082889760	0.85970854936307	−4.25730239989086
N	−0.08800341314423	−0.23134505224539	−3.64368710906168
C	1.08363371063447	−2.74592674406210	−3.06201242540785
C	−2.91799131592520	0.19768935279909	−3.43206953019306
C	−1.25711906117650	2.56539177707659	1.39218102975658
C	3.03377706904657	−0.20114317803353	1.52234188491570
C	4.98942665321742	1.18812622152948	0.89124308280982
C	−0.73038693831479	4.93580039760462	0.88506637413778
C	−2.67848808607559	1.89841829974073	−5.22906774762364
C	2.72511404883520	−2.29319542423720	−4.87545162519942
C	2.55383342249581	0.34953193793264	2.71023867479273
C	2.06533922830547	−0.46789344543931	3.71681496825662
C	2.05514182217509	−1.84772231639408	3.57488711977958
C	2.56616561062093	−2.39442019780184	2.41188837749716
C	3.04984896891808	−1.58536080247447	1.39304844233574
C	−2.47327742294345	1.93014382569299	1.17379725945372
C	−3.02537632585417	1.11022257298367	2.14983445057676
C	−2.38708975715365	0.90680211191192	3.35915486552310
C	−1.18776132433243	1.56536539856092	3.59070916623866
C	−0.62725935042847	2.38413057487700	2.62441200144999

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C    -3.72283969691003       -2.07288277263164       -3.67488089538297
C    -4.55758000554817       -1.89714179708467       -2.57559082387551
C    -4.58962302644422       -0.67414379333996       -1.93602473108904
C    -3.77391495574398        0.37072157841497       -2.35290768834104
C     1.35594467934309       -3.33602734290879       -1.83714557194779
C     0.49648866675020       -4.30363119309070       -1.32598092040997
C    -0.63353400056628       -4.68772060025941       -2.01649679947058
C    -0.90157100846192       -4.12386163557641       -3.26256907089412
C    -0.03967324379835       -3.16734162555341       -3.78107794007216
O     1.63861187155316        0.13030851739699        4.87410484166941
O    -0.54312233432242        1.47262691903040        4.79649199087966
O    -1.98640582758449       -4.61393201790803       -3.90827381273602
O    -3.81104812995159       -3.26913943603338       -4.31112999451597
C    -2.69400557947080       -3.88703355835284       -4.86683498235188
P     0.08642308506383        0.08281321838789        5.36394966767512
C     0.25135238471709        0.45127703294709        7.09713974123324
O    -0.63723338864383       -1.12258490456897        4.92746819636633
C    -0.73587222230051        1.18564852109220        7.75098909287771
C    -0.65798881732773        1.37912198002333        9.12006124136214
C     0.39738713057421        0.83980382404950        9.84039482425184
C     1.37961946536211        0.10590735713038        9.19200100603101
C     1.30943622212650       -0.09148687123765        7.82325805781987
H    -2.78407940665895        4.24883529816083       -3.79507111832778
H    -2.04019007484477        5.39314600478263       -1.47574317334425
H    -1.24945707150183        1.33739270319609       -1.28391480386068
H     1.72512205755140        4.87331443886001       -0.87955570026687
H     3.98247383385749        3.39099064253536       -0.82942825261462
H     0.91985365793342        1.25434232648476        1.04919859732548
H     5.84474614246194       -0.12436901030824       -1.38916753396285
H     4.97218847114177       -1.43527907463641       -3.57634306733997
H     1.77107879149509       -0.72989232510813       -1.06024288774400
H     2.36710875412626        0.62003519351317       -5.58972499537525
H     0.21360892272886        2.23228815913589       -5.73724102301492
H    -0.61841891643958       -0.89483727415212       -3.09681190037459
H     5.45272211748375        1.84901015722158        0.15866059456122
H     4.90740447678841        1.73231543579354        1.83037718173621
H     5.65232876126451        0.33921034202490        1.05464427289855
H    -1.77624878947761        5.20750928497272        1.02460858246661
H    -0.23034281671409        5.03024196394956        1.84680313605629
H    -0.27671074513601        5.65153261222115        0.20051631302625
H    -2.72886553641288        1.12616623153842       -5.99447803705363
H    -3.69281001485762        2.24200616836699       -5.03029088725901
H    -2.10585361631228        2.73429129391630       -5.63000849712356
H     3.36917188007753       -1.56955874929737       -5.37443622466825
H     2.01686642408269       -2.67165478723891       -5.60969539238266
H     3.33966927003320       -3.13014425068376       -4.54593538894802
H     2.57810023041690        1.42048929562804        2.87675324261258
H     1.66796713127629       -2.47903769066038        4.36174832474950
H     2.59176485699613       -3.46969481910095        2.29721270300052
H     3.47779152065535       -2.04478030808700        0.51168197143193
H    -3.02167197308104        2.09313334996129        0.25591144683579
H    -3.97251423483847        0.62306402830682        1.96174689824348
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H    -2.81746891001123        0.26176032829081        4.11126554325771
H     0.30011094812273        2.89525582617770        2.85778898577532
H    -2.29455677492104       -1.14016656587522       -4.98393902597556
H    -5.18618179934796       -2.71457071085528       -2.24886137023740
H    -5.25874288665202       -0.53122332865861       -1.09784368793373
H    -3.84044314991423        1.32984418134352       -1.85648740347594
H     2.25054275864179       -3.07901242521914       -1.28696969766103
H     0.71549091005926       -4.75886687600871       -0.36929219177897
H    -1.30643075327326       -5.43371589914856       -1.61527060828962
H    -0.21736097897341       -2.74500556552639       -4.76241649175901
H    -2.05519166724618       -3.18216704892229       -5.40622623227010
H    -3.08413177143065       -4.61360537379535       -5.57566861970883
H    -1.56221628871244        1.61446676120814        7.20046484852240
H    -1.42294562518534        1.95322521824376        9.62453404294363
H     0.45539051053138        0.99313748098921       10.90961586127855
H     2.20437668756692       -0.31273989047851        9.75192656079602
H     2.08506569057579       -0.66005331297540        7.32842322915871
Na    1.43356692739251        1.83176896222685       -2.47563331118817
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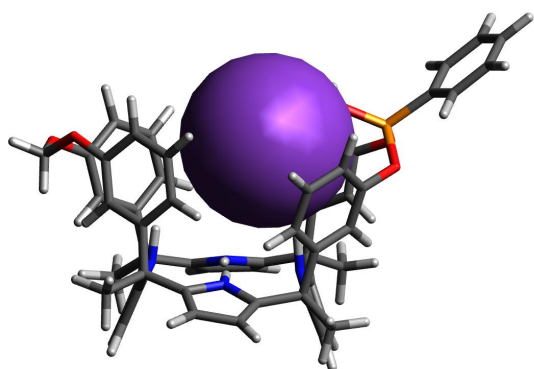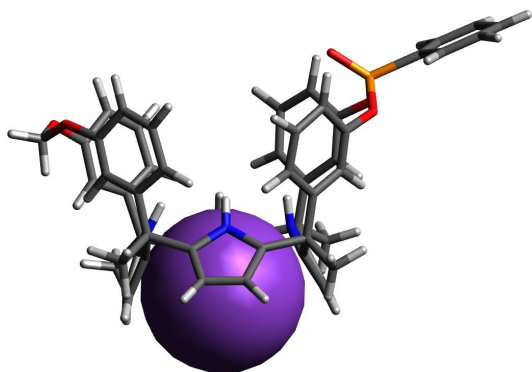
Complex **5** *(upper rim)*, $E_{tot}(Hartree)$**: -3653.773833393444**

C	−1.11211018495508	3.66353936590036	−3.98488841538210
C	−1.80937365021529	4.83580663908429	−3.85400662562342
C	−1.39241107322675	5.45189852738593	−2.64583672306616
C	−0.44620900960732	4.64271944940964	−2.07350844591131
N	−0.29491484587626	3.56070472612529	−2.89464771335196
C	−1.24818424642205	2.54160693338158	−4.98200888516591
C	0.24365122040687	4.72848401552275	−0.73872905077749
C	1.72307705504465	4.45383739454332	−0.88358591039752
C	2.75168332034421	5.29863464199569	−1.19292005761286
C	3.95553366047551	4.55017613245529	−1.15822954954572
C	3.64259527060860	3.26083040876596	−0.82856944974757
N	2.27051048548898	3.20159761061328	−0.71796202952996
C	4.53431398560455	2.05761008904866	−0.64108533564189
C	4.59462197490527	1.23883365447477	−1.90196640890547
C	5.62707070691108	0.53606033646285	−2.46358051074699
C	5.08540396289009	−0.26393295198540	−3.50398777456810
C	3.73851853870993	−0.02020602425573	−3.55468802714408
N	3.45510284127961	0.88203748779499	−2.56774081611104
C	2.65481496436899	−0.58594695558313	−4.43075223338427
C	1.84953636252394	0.54207832132690	−5.04004551495615
C	2.07512221535855	1.29022550157904	−6.16198076399538
C	0.97910853145343	2.17849425500709	−6.31995457565666
C	0.10874991706963	1.95583371161256	−5.28946490926886
N	0.67767754247125	0.99961298345604	−4.48185393188803
C	1.71918258899758	−1.51400374563222	−3.64364219741585
C	−2.17386173315353	1.43930782264383	−4.43013460677008
C	−0.38773612088299	3.74386457358235	0.25639401921792
C	4.04746317705294	1.16240844990179	0.51278609194578
C	5.94797167953503	2.53369075116862	−0.26957723514350
C	0.05025720101036	6.14321317614007	−0.17041424255974
C	−1.87372983009897	3.08991093116137	−6.27221534648504
C	3.30299974648494	−1.41647690133500	−5.54900407173451
C	3.46294078230060	1.71418467343316	1.65390199496162
C	3.11280156949870	0.90298245457005	2.72305189090457
C	3.35956557068132	−0.46136806203421	2.70907692177633
C	3.94289305336231	−1.01104635284572	1.57768022221934
C	4.26437832329024	−0.21584987160120	0.48603627187687
C	−1.56656395489678	3.06345396080687	−0.02908273335461
C	−2.16209150719271	2.24057828262791	0.91918842199087
C	−1.58910244582247	2.06460154504071	2.16730583342853
C	−0.40447281394705	2.73225729118756	2.44629425862685
C	0.19413267981729	3.56111940480079	1.51416032720491

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C    -2.20567600070789        0.18995775055608       -5.05396159306238
C    -3.04743069131352       -0.81179264916976       -4.58962032927751
C    -3.88012948734482       -0.58196575860898       -3.50329598198489
C    -3.87632716345906        0.66462813310428       -2.90604629534460
C    -3.02811106614301        1.66680883644527       -3.35744074746070
C     2.00491200276101       -1.97507151627389       -2.36497220225293
C     1.11693465153856       -2.84677779686576       -1.73691399622518
C    -0.06129447721298       -3.23977118182479       -2.34584252717656
C    -0.34998966325970       -2.78910948928321       -3.63640007797189
C     0.55176242405242       -1.94727833196993       -4.27315938245355
O     2.51135387048259        1.47836309366856        3.82211510599324
O     0.18477238802028        2.59730457260503        3.68810877236305
O    -1.49527806267300       -3.25321571950686       -4.17648200912727
O    -3.15427531211876       -2.03023430451378       -5.19821926443275
C    -2.01238966793506       -2.78911573604202       -5.39810204930655
P     0.93571371391035        1.22927441809942        4.09758134646385
C     0.82546706917648        1.22911006003373        5.86569378385027
O     0.42936546921102        0.06672225805909        3.31204724243242
C    -0.34842411132692        1.65548571903973        6.48638285209866
C    -0.46176682731184        1.58179575041071        7.86384212879164
C     0.58786005817293        1.08476771087556        8.62325647546035
C     1.75700771903693        0.66260170157605        8.00763446949411
C     1.87983804829411        0.73138193391218        6.63032475737815
H    -2.55667925551935        5.21357139109427       -4.53262869920578
H    -1.76577812433855        6.38088807318689       -2.24727002555223
H     0.44880130381112        2.88851611495016       -2.81730461393771
H     2.66359113014212        6.34716465338989       -1.42600377201773
H     4.94138150997060        4.93307279094340       -1.36323146842668
H     1.79117014670596        2.47008895623502       -0.22228100319011
H     6.65896800992705        0.56076367621409       -2.15276148403813
H     5.63905654304420       -0.94158372551618       -4.13268261831450
H     2.59283627122176        1.39776074471127       -2.51702089006809
H     2.93095565550771        1.21949458291281       -6.81341007900646
H     0.85364360607899        2.89772584682414       -7.11220357878259
H     0.13089467159164        0.45761525879089       -3.83130758285104
H     6.39180363204563        3.10544650493191       -1.08369252488289
H     5.91882703530585        3.16220603824181        0.61938048359397
H     6.60295901072805        1.68891316274271       -0.05881942031246
H    -1.00759519043464        6.35429871738770       -0.02080592586912
H     0.55281070713578        6.24934774897496        0.78931786922346
H     0.45602426042305        6.89191734450302       -0.84895859985303
H    -1.93426610217720        2.31226278856633       -7.03186121327242
H    -2.88478546843773        3.44962553122070       -6.08611258420292
H    -1.28882487203069        3.91873541074095       -6.66985208410786
H     3.98484172097469       -0.81178770931197       -6.14576222439871
H     2.54638362253503       -1.82895962750180       -6.21388667771470
H     3.86491718193168       -2.24917090405684       -5.12707012367871
H     3.30807351339767        2.78381910333149        1.73161578499995
H     3.11147000135127       -1.07858613982159        3.56281789810033
H     4.16466589148880       -2.07056675620153        1.55291590635342
H     4.72836645943808       -0.66857479648652       -0.38026504650821
H    -2.04604403447803        3.19987870335055       -0.98683552656230
H    -3.09738914073035        1.74872854339457        0.68500204356214
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H   -2.06480267957923      1.44418085785260      2.91494527046065
H    1.09898062390896      4.09176608472279      1.78804198918446
H   -1.58389989679710      0.02108040699960     -5.92677243013548
H   -4.53741247387237     -1.37018816979786     -3.16113939930560
H   -4.54887007695882      0.86155769674347     -2.08106825941548
H   -3.06060226438202      2.64185127502155     -2.89131905804273
H    2.93539507823175     -1.70460611219548     -1.88415594188431
H    1.37655848277561     -3.27039551063376     -0.77121546885561
H   -0.74220258215300     -3.92768761411620     -1.86133078166187
H    0.37463587521784     -1.60545572097820     -5.28358508650552
H   -1.25771290532274     -2.25595573266063     -5.98188797514592
H   -2.33376276269329     -3.66322007995119     -5.96133600674072
H   -1.16906304248549      2.06047127434562      5.90942735721430
H   -1.36905928297595      1.91923254078254      8.34537636404681
H    0.49648237769654      1.03252054846657      9.69978734568491
H    2.57861979572567      0.28347767210044      8.59974227660287
H    2.80269677206098      0.41248192281056      6.16508443907315
K    0.52370753002451     -0.56322307513200      0.82903373551395
```

Complex **5** *(lower rim)*, $E_{tot}(Hartree)$**: -3653.783828586929**

```
C    -1.77376314105564      2.47646685988504     -3.01333157643553
C    -2.02160805813315      3.91492329348729     -3.09098100542533
C    -1.63874381817119      4.41057489724575     -1.87250028319408
C    -1.17168991045229      3.34764194644894     -1.00068443654977
N    -1.31438967908313      2.12165108925316     -1.67370553869523
C    -2.07374981675348      1.29515233385886     -4.05142718237292
C    -0.58741427005649      3.63018806133578      0.33374580756467
C     0.85980452421327      3.20397266871466      0.17791226978566
C     1.87560948988902      4.09264708623266     -0.01453768729589
C     3.12299092810027      3.35396270541778     -0.00927285702102
C     2.80501969996115      1.97180779793534      0.09797726595219
N     1.41410056036280      1.90484198036811      0.23749678429261
C     3.69171569282005      0.80963573712523      0.56215689363542
C     3.53630310765363      0.15625426644501     -0.78562601212877
C     4.61189387369883     -0.03291780162394     -1.86171703386404
C     4.15840248962100     -0.73942999195365     -3.01512073507549
C     2.82849480410693     -1.00988896671272     -2.71436839831730
N     2.52838576147091     -0.65693705967011     -1.37998080419661
C     1.82796606979179     -1.80249096250842     -3.65103282956277
C     1.15963763024725     -0.55129564996679     -4.18773610733795
C     1.28514759925565      0.21464169386761     -5.35382020726865
C     0.13807674604779      1.03892098533629     -5.45717373325268
C    -0.71013346930021      0.68382281529561     -4.40475460037039
N    -0.10048675509766     -0.32102111063580     -3.76259592370833
C     1.04420121794637     -2.91899785423080     -3.04402483440170
C    -3.06452608451957      0.15689498358658     -3.56963578950065
C    -1.14095661571373      2.71558827910767      1.43910570375859
C     3.15154621384002     -0.12133722213348      1.61621095894752
C     5.15476815518642      1.29019043878515      0.75682502185345
C    -0.76893178858373      5.00927788492412      0.78431494718582
C    -2.57986055977862      2.05134331394156     -5.35699600313109
C     2.83183027343048     -2.35611137586014     -4.76483086339498
C     2.53968304792393      0.26697693606102      2.77688653809242
C     2.12892206352128     -0.64944123805568      3.70323881157164
C     2.13155506560353     -2.02916759797523      3.57843274940036
C     2.73802276802064     -2.37678454622296      2.42226223660744
C     3.14218455883541     -1.48537026699850      1.41617078950268
C    -2.37331752281840      2.10233357558337      1.25504015765311
C    -3.19723009001674      1.28661288869137      2.15653468770353
C    -2.57308592113836      0.90996415289288      3.34449943183060
C    -1.36199078998780      1.50333056238858      3.62251497731741
C    -0.63563445183561      2.33107530406095      2.70763515153173
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C    -3.06144419350084    -1.06001169018016    -4.22798276775747
C    -3.88707668701062    -1.97744282688350    -3.67762408906631
C    -4.73329530636249    -1.72298489265412    -2.50754566502874
C    -4.65600204063405    -0.49625312534259    -2.03357248703543
C    -3.72155179283919     0.44409731297461    -2.50098176934931
C     1.53359310006810    -3.43252637505088    -1.87129235316770
C     0.67960958307492    -4.48896843713413    -1.36744094159778
C    -0.46178167001863    -4.86710535717409    -1.82901886572736
C    -0.79576181745222    -4.26927439007210    -3.06486720273159
C    -0.13742967585720    -3.31561156150568    -3.59138249431169
O     1.45944134998925    -0.05771587112133     4.77924249799470
O    -0.71965421104594     1.28888694307569     4.82930437207131
O    -2.16700469263376    -4.45880784985277    -3.69348684696280
O    -3.98390581834104    -3.27762256596511    -4.12117361886711
C    -2.79942519151441    -4.02812506585454    -4.66549043892696
P    -0.09051545455693    -0.10030830213829     5.31228959710584
C     0.08213203871925     0.27658830061022     7.14028613730362
O    -0.81774448279096    -1.30553545072728     4.76871886790318
C    -0.85020657457330     1.04632920209240     7.77085204228182
C    -0.66604320115089     1.29052655271676     9.12472663857573
C     0.52029852688130     0.94667362277005     9.76888444000454
C     1.37586009524610     0.09001746563576     9.12849920938290
C     1.25897998044632    -0.19368460178186     7.79864990749612
H    -2.48497797416591     4.41170787679196    -3.88146627762748
H    -1.75700906094278     5.38961908901117    -1.60129687982794
H    -1.34861575667144     1.24629067208035    -1.12005001254229
H     1.74494948782386     5.17861627720366    -0.16800795326950
H     4.21586880786301     3.59924463932171    -0.12380120896912
H     0.87046990677844     1.25667849630158     0.70273793972695
H     5.62568227700819     0.27494937000308    -1.67069310379319
H     4.76673571281381    -1.05254469644906    -3.84794436583847
H     1.71487569073848    -0.92452507727916    -0.88789118162765
H     2.22292927336917     0.14450017592862    -5.90718893867264
H     0.07688341515666     2.01033746569308    -6.03583130404531
H    -0.43366519914817    -0.64008796739772    -2.81986434137025
H     5.41832753634146     1.95007444933477     0.03078586907811
H     5.09313170159136     1.50139815980247     1.85990310521465
H     5.78537803110871     0.41614613667229     0.88073265227402
H    -1.80118615734529     5.13254809679530     0.85249845166679
H    -0.39109009025086     5.14881633792344     1.76891325370861
H    -0.46313617602706     5.63808920922049     0.07996738643098
H    -2.69722306900148     1.24153082506222    -6.11861168263963
H    -3.62745079273001     2.41623237782363    -5.11691980992784
H    -1.98621388180284     2.87512670882415    -5.54734676573942
H     3.30533455164719    -1.48614215022389    -5.33392501194886
H     2.13062675698390    -2.94169397893909    -5.40448501329008
H     3.52750288009606    -3.08874985448225    -4.44471848889092
H     2.51818219586238     1.28839449026152     3.01417513244666
H     1.74018855637852    -2.66640748072015     4.31435995691370
H     2.77943005376189    -3.36645802967997     2.12663778515933
H     3.65639068326921    -1.88983784258170     0.50946441169922
H    -2.88242046686137     2.27787451458264     0.36883898960416
H    -4.16521923929111     0.81454599815792     1.83612454422432
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H    -3.01406502125315        0.31953183655874         4.12962052949123
H     0.28959459321094        2.74218667916479         3.00806577099329
H    -2.42520175158406       -1.16607298840879        -5.09573640706251
H    -5.37572924332713       -2.53141821141758        -2.19252738142681
H    -5.15939393377085       -0.34344098245246        -1.18449125107679
H    -3.67385316601083        1.38469538406430        -1.97476182266245
H     2.43813228662900       -3.05364794690525        -1.45498593190043
H     0.91102532218658       -4.94977542623633        -0.52079409409333
H    -1.12833546709518       -5.61581473606389        -1.42255305239485
H    -0.41713841802267       -2.76848698466826        -4.55720550476277
H    -2.12372817063909       -3.36886737486655        -5.21665835754950
H    -3.01677469427643       -4.79656594005580        -5.36390135483113
H    -1.73153988890983        1.43977996661043         7.18833338349711
H    -1.34612389237733        2.02122595199962         9.53868567937435
H     0.61994441891378        1.16587470557351        10.75641251638695
H     2.31185819290677       -0.14930443355543         9.58671717484794
H     1.93852548217727       -0.83122549442683         7.28116309336350
K     1.79379182535895        2.03983583005988        -2.81367089602249
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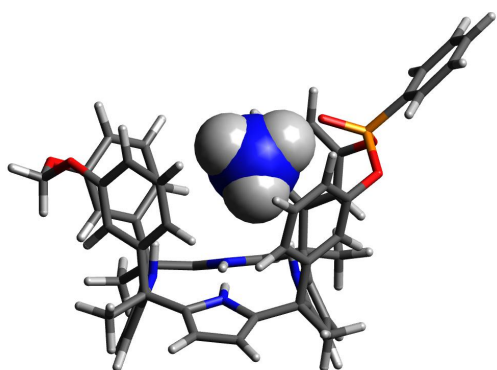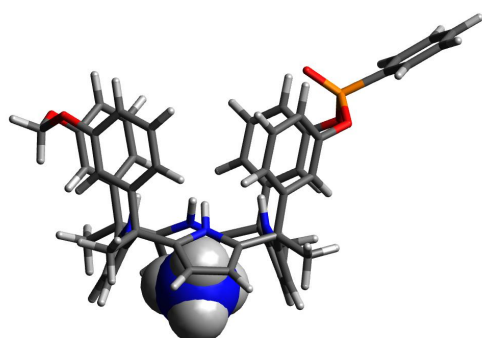
Complex **6** *(upper rim)*, $E_{tot}(Hartree)$: **-3111.284661592777**

C	-2.54611703681062	3.04919252965871	-4.12913671430528
C	-3.53186279879217	3.98079195278985	-3.93345445799822
C	-3.21951938302925	4.69372518703367	-2.74728112645090
C	-2.04617920173110	4.18561028104634	-2.25435690071059
N	-1.65567171622043	3.18665599792186	-3.10146943698382
C	-2.44390666325612	1.91504235173390	-5.11590742006280
C	-1.32028100671468	4.46543867058738	-0.96589716742743
C	0.16318981935704	4.63585014461416	-1.19961874266803
C	0.88815210904437	5.74949810684385	-1.51724908724816
C	2.25715822607638	5.38021745318293	-1.56411792978609
C	2.34432329599898	4.04719145254929	-1.27718490596939
N	1.05540698897681	3.59028891584205	-1.11008030336178
C	3.54605734918292	3.14151086662055	-1.18228578748900
C	3.73318583864069	2.36974199112294	-2.46010951203547
C	4.87376635595403	1.98016814015325	-3.11041729515634
C	4.49871202250724	1.04561366292792	-4.11097108213164
C	3.13936236966652	0.89438159080183	-4.04729423202076
N	2.69135755429428	1.69577648046635	-3.03468586925210
C	2.20021323734721	0.02025361333153	-4.82980738291582
C	1.07155294578320	0.85435710084349	-5.39707102426374
C	0.99187806726507	1.57515745322533	-6.55601232614952
C	-0.31855561186528	2.11756933095853	-6.64225229649930
C	-1.00869006237198	1.71628007308024	-5.53312944000026
N	-0.13444338320052	0.99950703027342	-4.75003831360343
C	1.62618605337385	-1.10390980498878	-3.95579971863661
C	-2.98699875897696	0.61608585381205	-4.48651037395865
C	-1.56539959934230	3.34045009644579	0.05092821381106
C	3.41108564304228	2.14757256154609	-0.01506089275323
C	4.79645865617669	3.98706071836507	-0.90471441816994
C	-1.88485602284658	5.75862370054004	-0.35414597130236
C	-3.29902507094904	2.23663344640128	-6.34848873543357
C	2.97366495717298	-0.63949609136954	-5.98156728555052
C	2.78461391935391	2.51853933106281	1.17581006286102
C	2.75113212891945	1.64051504658634	2.24764321307966
C	3.35791409660909	0.39686282410014	2.18782209801309
C	3.98474129361772	0.02849537238172	1.00905211312194
C	3.99472805955232	0.88170696158011	-0.08568658064753
C	-2.49848396073767	2.33149381998214	-0.16776802799174
C	-2.76733496414714	1.38361273671615	0.81316373108195
C	-2.10013365736501	1.40748190790644	2.02619764583732
C	-1.15029364770000	2.39760329614031	2.23160572655470
C	-0.88144499557419	3.35422564068460	1.26979854872390

S47

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C    -2.69340388448588    -0.61865769225657    -5.07136165244052
C    -3.20804311614191    -1.79410849090574    -4.53814687853851
C    -4.02937061609161    -1.75679656160920    -3.41974422880424
C    -4.34650785278951    -0.53436562183616    -2.85807360306199
C    -3.82685425918827     0.64220790671894    -3.37885604395396
C     2.14338228690950    -1.43837093417448    -2.71160973152693
C     1.59905666212991    -2.51050371434060    -2.00749480442324
C     0.53006911280482    -3.23191113730921    -2.50529835143674
C     0.00890753869721    -2.90762327516835    -3.76017045115197
C     0.57246923497345    -1.85876042313103    -4.47323374192418
O     2.08894684479139     2.02032332143034     3.40030151227280
O    -0.45880535246060     2.44957453269437     3.42921996206375
O    -1.00333595362445    -3.68858064007980    -4.18990628720367
O    -3.00680263668101    -3.02107178675553    -5.10365234260045
C    -1.71658033029128    -3.44809319036954    -5.37581805099368
P     0.66795868622272     1.35201816667450     3.77196284143031
C     0.67426727065537     1.28332400118781     5.53879577458896
O     0.45493082144010     0.08094855673005     3.00723599481605
C    -0.48160091329932     1.56600541251868     6.26488835928373
C    -0.47156878248874     1.43624443356071     7.64355184437998
C     0.68044240396238     1.02268463045440     8.29597100974532
C     1.83083027368031     0.73854678635500     7.57339461979224
C     1.83275789333798     0.86831451372719     6.19593165829098
H    -4.40201651041493     4.12413346327369    -4.55309415535197
H    -3.80977475165930     5.48136117219827    -2.30841195114579
H    -0.74727809887252     2.75594376380372    -3.09476459503825
H     0.49331363528163     6.73457379350508    -1.70325762718034
H     3.08049464310440     6.03763914608802    -1.79008868918084
H     0.83852316650999     2.74084587633347    -0.61815820737651
H     5.87848376370887     2.29787795430037    -2.88369386123657
H     5.16648973933150     0.54286013234379    -4.79074145866296
H     1.72561612804805     1.94649661172643    -2.90790571368880
H     1.78173037432583     1.71072822975344    -7.27716765642706
H    -0.69998532983782     2.72900384540797    -7.44373347601595
H    -0.46438379536697     0.34644405224596    -4.05644546790552
H     4.98240733387402     4.68181997030455    -1.72271667526084
H     4.67882310012492     4.55937150085952     0.01445451211018
H     5.67412298032722     3.35253139959323    -0.79437979365222
H    -2.93202618884735     5.62924085183074    -0.08498778672345
H    -1.33695347652939     6.03591621375782     0.54424636256984
H    -1.81705547288103     6.58431944372468    -1.06075559878298
H    -3.22012475879429     1.44184929507175    -7.08820671647452
H    -4.34803505131564     2.32808927069567    -6.07167518286877
H    -2.98654021027232     3.17367060016904    -6.80779127560323
H     3.44736746019542     0.10843210510912    -6.61562937526594
H     2.30547858496260    -1.23244134192495    -6.60246250240063
H     3.74875697809356    -1.29825370094935    -5.59229922066009
H     2.35055392184733     3.50559444086791     1.28410232989405
H     3.34480144756277    -0.26850817161641     3.04048062848557
H     4.47843946632630    -0.93250449130872     0.94337212334591
H     4.50076973539850     0.57241735985747    -0.99105865310303
H    -3.05438495833899     2.30093971679501    -1.09324275507240
H    -3.52124690788437     0.62835271797831     0.63260770037876
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H    -2.32204605309465      0.68301122429556      2.79825181056763
H    -0.15418976901706      4.12971893468251      1.48202885415374
H    -2.08070892424870     -0.64775036436506     -5.96673868334806
H    -4.43066634782578     -2.67981313343203     -3.02320407599465
H    -5.01684261607332     -0.49511299572454     -2.00890628585452
H    -4.11181259593223      1.58941245259346     -2.94198992967285
H     2.99759928509570     -0.90588972057222     -2.31586833346057
H     2.04892349050787     -2.81330768386308     -1.06742503899564
H     0.11838414472815     -4.07262922224816     -1.96190696339386
H     0.21216644298422     -1.60249643825217     -5.45979952524124
H    -1.18581790426603     -2.76423665375475     -6.04392452891985
H    -1.82626477466596     -4.40695258138991     -5.87882122366187
H    -1.38262894627478      1.90050578739337      5.76974546872406
H    -1.36353014067057      1.66591542576601      8.20990519038922
H     0.68408028755296      0.92670197681988      9.37341319846062
H     2.72974984774735      0.42237304921643      8.08425278558558
H     2.74054946479389      0.65792485994625      5.64557455276959
H     0.47611022674296     -0.16079976186745      1.48170949093969
N     0.46473902076959     -0.28918690961098      0.41088089540572
H     1.32495560953581      0.08307633691215      0.00337398647878
H    -0.34784512974240      0.19642082105565      0.02922789100664
H     0.40174988696752     -1.27236100798974      0.15059795489577
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Complex **6** *(lower rim)*, $E_{tot}(Hartree)$: **-3111.293355423948**

C	2.32918573768155	4.37119227543786	-4.36160733540941
C	1.30179552707278	5.19269276039062	-4.73736654868836
C	0.33289967462763	4.39922643160308	-5.40512996600089
C	0.78918654968648	3.10991593223998	-5.42314348690168
N	1.98740762852098	3.09698183447201	-4.74995900927923
C	3.59214108175443	4.67684349444758	-3.59586504140669
C	0.17120785909175	1.85945024249346	-5.99697373451732
C	-0.19104176918961	0.94577752230398	-4.84608067774634
C	-1.34506344453630	0.87291155514759	-4.10095714448756
C	-1.18208139556903	-0.17346158931989	-3.15344555004682
C	0.06728674086747	-0.70807563524772	-3.33433568682360
N	0.66886368393478	0.01055070796131	-4.33550649943684
C	0.77350619423397	-1.81246443898749	-2.58043069240143
C	1.49510506564809	-1.18887314910412	-1.41207602371864
C	1.29176301083201	-1.31637147932498	-0.07071920907475
C	2.26957051766291	-0.52497282139336	0.59944514786093
C	3.04832756256505	0.06986592527741	-0.34668734655906
N	2.53177116276585	-0.28338288060321	-1.58403596159320
C	4.21378293820992	1.01597504738224	-0.20661666564503
C	3.77544512161854	2.36624729787546	-0.72493130317146
C	3.17182947956846	3.42025490771268	-0.08820319781919
C	2.98506773396220	4.45360493918726	-1.04753157665754
C	3.48615032009438	4.00318045975134	-2.24662406372465
N	3.91055624726627	2.71953796994852	-2.04136274196522
C	5.44902195203526	0.52299242455743	-0.96738133839244
C	4.85230514191982	4.20275746465796	-4.32830348371788
C	1.10894475620269	1.16060130449380	-6.98498037851220
C	1.73401892151924	-2.57734464665978	-3.49301831135707
C	-0.26725890887987	-2.81262680556042	-2.05856281964804
C	-1.10556660905049	2.23293711610481	-6.76455620629226
C	3.70222403537455	6.19514259917601	-3.40102673920801
C	4.58946874777453	1.14064897143300	1.27588707208906
C	1.34349812731573	-2.89329744096278	-4.79295644629557
C	2.17940118787880	-3.62575599141202	-5.61863810806925
C	3.42070943827367	-4.05781936187687	-5.17560513514023
C	3.79317105967766	-3.77315989817964	-3.87435427753500
C	2.96107289599495	-3.04410219484843	-3.03582279810951
C	2.12790627116196	1.85095874150049	-7.63139874711559
C	2.92885605090694	1.21101581595056	-8.56696634257859
C	2.73234912943255	-0.12157792657214	-8.88151817735556
C	1.69291300172681	-0.80068361458101	-8.26406116906312
C	0.88856349544987	-0.17294470753075	-7.32736780357683

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C    6.05091524944298      4.08891050670599     -3.61865919417388
C    7.21831431534407      3.69384671415140     -4.25739771418424
C    7.20193656273064      3.41963234685160     -5.62181328648869
C    6.02658166947323      3.56806601159713     -6.32988674659977
C    4.85307083130834      3.95463560612605     -5.69352152846554
C    5.61499520134271     -0.81204241574260     -1.30394446542563
C    6.76843307927439     -1.22112805937150     -1.96415194744349
C    7.75602060261672     -0.31729873337014     -2.29564247518560
C    7.61390799185024      1.02100510838067     -1.93343858878172
C    6.46858741522321      1.43142067063791     -1.26487305828148
O    1.71989694545554     -3.95395898617230     -6.86730167744151
O    1.39593769156700     -2.09653459448059     -8.60145801752710
O    8.66644627490517      1.81924506929020     -2.22934189580604
O    8.42986841656415      3.61657682952628     -3.64889804106246
C    8.57159788117530      3.20810985705618     -2.32564994770549
P    2.36908292748182     -3.34715736280681     -8.23066416708553
C    1.86255270313742     -4.55849538565790     -9.43394563267512
O    3.78784658460398     -2.97767606011374     -8.10368335497059
C    1.62996117758677     -4.16534622799301    -10.75062916307864
C    1.34471126632503     -5.11654206819700    -11.71559031414038
C    1.29264946489625     -6.46000678790712    -11.37408006237966
C    1.52570356250696     -6.85453687399628    -10.06511727371712
C    1.81256358094641     -5.90885695192027     -9.09457963226026
H    1.23726773440929      6.25393891815010     -4.56229977639297
H   -0.59193955283461      4.75384271088249     -5.82860507360843
H    2.64470767544722      2.33601878639787     -4.80327321858886
H   -2.23395855601686      1.46518401300345     -4.24775023786326
H   -1.91827860399654     -0.50614843248723     -2.43932408462289
H    1.50770645163515     -0.28907265900415     -4.81093135864193
H    0.53018671676758     -1.91245179258489      0.40462014397806
H    2.37390998402695     -0.41880340037197      1.66678226135993
H    3.11652460602962     -0.29760280686972     -2.40816315413649
H    2.91489819836334      3.47018248714515      0.95767717337787
H    2.58243565326357      5.43500373845965     -0.85445356313962
H    4.50544415583004      2.22594045099404     -2.69006827769519
H   -1.00009596633481     -2.33308746069822     -1.40998827693963
H   -0.79988942859196     -3.26659514761664     -2.89178455618447
H    0.21910873799060     -3.60815765597419     -1.49619590539222
H   -0.86416895909489      2.88882478092865     -7.59942276877182
H   -1.57949263643522      1.33856157212843     -7.16394377836136
H   -1.82849597218977      2.74316221850716     -6.12882285495224
H    4.58557487921698      6.44387448918190     -2.81589441875278
H    3.78783208772891      6.69299720158446     -4.36567521807376
H    2.83126867968020      6.60060560390257     -2.88637274088371
H    3.75218060886529      1.49733153788313      1.87558852460682
H    5.41033274558120      1.84462109874472      1.39686289622524
H    4.90773974047285      0.17722828837103      1.67078503538822
H    0.37109426982791     -2.59571256264086     -5.16889280221013
H    4.07384381197254     -4.61783607619540     -5.82945866161585
H    4.74650287804302     -4.12745393410372     -3.50605995966986
H    3.26230686821826     -2.87004759763547     -2.01103220666644
H    2.28386223784785      2.90279654852101     -7.43225474891611
H    3.71856346637107      1.76306284921829     -9.05851544904964
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H    3.36488592362225      -0.62028195081972      -9.60229666877120
H    0.06760240517411      -0.73135876188523      -6.89296530519306
H    6.06334911331778       4.34807869406745      -2.56714517381750
H    8.11558164865303       3.11186827613883      -6.11221333785778
H    6.01899842610426       3.37605358171267      -7.39447149152414
H    3.95156686333605       4.08675891235232      -6.27562736264072
H    4.87135482221766      -1.54656612225838      -1.02497561415952
H    6.89508781902108      -2.26332625892879      -2.22540838976084
H    8.65017899331542      -0.63412422353210      -2.81538594172032
H    6.35723717281946       2.45684628567189      -0.93647915718666
H    7.79097877062010       3.61577423054146      -1.67770431721999
H    9.53196998007893       3.59972944001565      -1.99966819503106
H    1.66069870362613      -3.12039442911378     -11.02945657449852
H    1.15974946342415      -4.80822012042657     -12.73550075588195
H    1.06946778214909      -7.20111818974950     -12.12994158426273
H    1.48317861830640      -7.90173110363518      -9.79823231489061
H    1.98873505151166      -6.23027854858646      -8.07700507098027
H    1.35468935530031       1.41577646143096      -1.90786746572097
N    0.70338516675009       2.21309304550197      -1.90219777305217
H    0.07923135958250       2.14564030327354      -2.71716860536196
H    1.24200409060052       3.08922246333359      -1.92146919828314
H    0.15668180998749       2.16562233146540      -1.04690450995322
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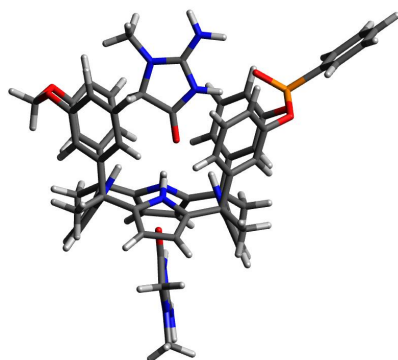
Complex **7**, $E_{tot}(Hartree)$**: -3845.837577751655**

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C    0.98763272538920    6.12467826940699   -1.66450319842882
C    2.17161955910700    6.33999490610740   -0.99344604585807
N    2.79005164594869    5.13041758568810   -0.89369081270122
C    2.49809649173525    2.69817086771776   -1.53336822545267
C    2.75642397065441    7.61399349679769   -0.42831452982627
C    4.00729610517206    7.98766085933800   -1.19328759569190
C    4.17801640208290    8.82245588567201   -2.27032470326970
C    5.55842224661237    8.82366993822133   -2.59695941043001
C    6.19641968097728    7.98681243522519   -1.71310321395373
N    5.23775070249660    7.48450525493204   -0.88423572737709
C    7.65991815499900    7.61957810989880   -1.59234160889364
C    7.93182612902787    6.32214744329678   -2.31837072839154
C    8.65788839926594    6.08185323714986   -3.45872588258093
C    8.60759920995443    4.68865032280955   -3.71424709016871
C    7.85106740317789    4.11087000358040   -2.72531042391709
N    7.46481027330067    5.11500683793526   -1.88537195650384
C    7.41653510763534    2.67331643801869   -2.55457732518517
C    5.93887310589175    2.55382119319145   -2.85041703137527
C    5.27254387369472    2.18332428541334   -3.99049000905516
C    3.88387154356272    2.19749054966704   -3.69998548801186
C    3.73601963483762    2.57505478049597   -2.38951053193288
N    4.99078384654346    2.80394409067345   -1.90290205123695
C    7.72407054105736    2.11717911623236   -1.15660767980187
C    2.73428015060274    2.11847746480241   -0.13146216414517
C    3.04447716716341    7.47825757995635    1.07068254592978
C    8.09582114609191    7.53720950949964   -0.12539497589403
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C    1.72033534542700    8.73999234427261   -0.57365291205333
C    1.37443910432848    1.86062002846514   -2.16496855987283
C    8.19987594519190    1.80100645287734   -3.54843032533946
C    7.56039566498212    8.40730332043777    0.82285736520550
C    8.02238869391854    8.38370064754250    2.12672563321304
C    9.02599628399532    7.51763251577828    2.52571029577109
C    9.57463393117416    6.67007406363087    1.57758902048618
C    9.11383801231166    6.67382420198426    0.26960885865063
C    2.37423303982026    6.55101643321932    1.86139295195232
C    2.58391908276290    6.50622503096801    3.23238498873475
C    3.47004643712941    7.37680184192308    3.84381217823394
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C    3.91995098309830    8.36951528263431    1.68898256489649
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C     2.99924907454642      0.88101440907156       2.36032815582039
C     2.14226741787674      1.95381639868425       2.19383203593470
C     2.02010189506346      2.58853859983208       0.96400693398428
C     8.72658612453081      2.65488210039199      -0.35869254214253
C     9.06816884901945      2.03866984167475       0.83926971692526
C     8.40022717788127      0.90873188213374       1.27625805920667
C     7.37994438102669      0.37031527239379       0.49289097392022
C     7.06246143679879      0.96431912369565      -0.72126808012323
O     7.48983887140418      9.28739184110326       3.03194072302116
O     4.97635476984659      9.23195826888363       3.63423662866484
O     6.79626523490021     -0.75504949704606       0.98123364014550
O     4.57238192071352     -0.61739835804521       1.54911198870715
C     5.50205063154202     -1.14809469016706       0.64389841013928
P     6.44475512666505      8.85141686969061       4.17016446775426
C     6.72891406280484     10.00671634916667       5.47793385592735
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C     5.67811626749534     10.36817616488335       6.32152288193486
C     5.91941340171778     11.20568039113234       7.39664489967124
C     7.20115655189651     11.68238162279336       7.63297610776006
C     8.24653874579816     11.32577708163736       6.79337794075451
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H     0.21675125590849      6.85781520827894      -1.84112247494293
H     3.70015410480423      4.99567823664204      -0.48636756319031
H     3.41247313379525      9.41252799677412      -2.74810548318379
H     6.02903085970713      9.42085181504851      -3.36151363108486
H     5.42393536540383      6.87982677950835      -0.09812447050733
H     9.20757120869657      6.81095867008696      -4.03166465231653
H     9.09664401493115      4.17497543468774      -4.52528037290788
H     6.84965201364078      4.99114739889191      -1.10039863848919
H     5.72269933727479      1.88536493038755      -4.92311694376710
H     3.09311207437779      1.91250939542994      -4.37498354621746
H     5.20078369988435      3.02839689399319      -0.94564387028273
H     8.27850756826679      8.83883951458031      -3.29753600091652
H     8.30295866893365      9.68706343129956      -1.75202082350478
H     9.56369943348414      8.51443602961024      -2.13590830422868
H     0.80994508263217      8.48817636689202      -0.03188225099251
H     2.11012375686773      9.67063877895760      -0.16675153672258
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H     1.67863996831717      0.81854536755935      -2.23838665108218
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H     1.13202680649104      2.21304279901406      -3.16704592368728
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H    1.33316449671458      3.41717357974073       0.85271308206040
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H    9.87581945045362      2.44216373000117       1.43626070502632
H    8.67775428705390      0.41695510547099       2.20010693881284
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H    5.47905964082745     -2.22641222625724       0.78382353549425
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H    5.10461463208403     11.49392449635811       8.04651966344585
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H    8.83737617476471     10.23040335136772       5.05974366386401
N    6.12658924311269      3.02046122475916       3.66699876730352
C    6.34951076725761      4.24923447164623       4.08936744259122
N    6.17667049375305      5.14504761465564       3.08579797730920
C    5.82601307237432      4.50906108357415       1.93004968147897
C    5.77648175319062      3.04574032713836       2.26127594286044
O    5.59758895903113      5.01986389493472       0.86108374740714
N    6.69355767722920      4.62671670239954       5.29811830913200
C    6.25168148236482      1.80781607488650       4.44802369047170
H    6.79771992562392      5.62029813088476       5.48220464903121
H    6.83703411058952      3.96893662929723       6.04537153097579
H    5.86944928617914      0.97602452803161       3.86211132543974
H    5.65960700938795      1.86731550359367       5.36161932900803
H    7.29224412969725      1.59660946468096       4.69464525278385
H    6.49313611113854      2.48174843603805       1.66101854474954
H    4.77484139607573      2.64592945031793       2.08801323251929
H    6.27908470177202      6.15752790336137       3.27561455108646
N    4.08430520328410      6.77091780973480      -6.07079836229416
C    2.92584960884667      6.69321200262481      -5.43932943620147
N    3.06670684901359      6.14897264482476      -4.22228988915039
C    4.41611766061520      5.87751593508139      -3.96351722347307
C    5.15092456478799      6.25825509682429      -5.22688433599064
O    4.85383075734949      5.43792062400881      -2.95520231005489
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C    4.27476006105305      7.28762592090909      -7.40914441707793
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H    5.31849235921434      7.16502983417504      -7.68265747926257
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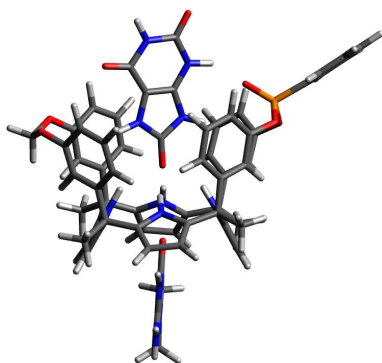
Complex **8a,** $E_{tot}(Hartree)$**: -4086.556288284895**

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O	4.51981259528998	-1.87644083629730	-5.86768841732223
N	2.25207769916956	-1.83238099816897	-6.00091159715842
C	1.15810502496280	-1.07920888721180	-6.24197647561494
N	-0.14848100365663	-1.46253022920843	-6.19452527735646
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C	1.19440014793845	0.22640576290803	-6.60082528183927
C	2.43661096338843	0.91062644090388	-6.78902707815940
O	2.60100416860839	2.05963108224216	-7.12476757783319
H	4.42990899213897	0.45730370949594	-6.63752726794305
H	2.15060139100350	-2.75032194272777	-5.56639415700531
H	-0.48634066586419	-2.37173011759025	-5.91519830016689
H	-0.41697463584885	1.56328341110491	-7.01688375851837
C	-4.63447792548854	-1.20937681973016	-9.53480888190185
C	-5.65437818035186	-1.98296607185106	-10.03631955229364
C	-5.85281442849822	-3.06051733000129	-9.13704310969093
C	-4.95032111017889	-2.91489836355995	-8.11107464953836
N	-4.21830440506473	-1.79768162212082	-8.37989373913629
C	-4.09592533831337	0.11429370761197	-10.02411022741302
C	-4.70395587719637	-3.77481687306691	-6.89498586992385
C	-5.07086045414244	-3.02255148619781	-5.63483774915449
C	-6.20204716395615	-3.07988095764696	-4.85610101711025
C	-6.02371863510934	-2.18042720776663	-3.77371377002004
C	-4.78730077635733	-1.60048084777729	-3.91876315897462
N	-4.23508198237018	-2.12024897213339	-5.05032386597967
C	-4.06625385488715	-0.58343306811600	-3.05927859326836
C	-4.40129137218803	0.80697419798423	-3.54447900699907
C	-5.20748433070281	1.76759716931004	-2.98161969896756
C	-5.25124046292134	2.86760403676222	-3.88198950348412
C	-4.45652522284705	2.54874193769551	-4.96462456841586
N	-3.96174984246184	1.30226924161547	-4.73618208972946
C	-4.12919965209821	3.34989350795031	-6.20332570559362
C	-4.68190266316447	2.65942240047499	-7.42760180820951
C	-5.79574356140157	2.91311727336527	-8.19210346527630
C	-5.78305881470874	2.00084557585551	-9.28146575356163
C	-4.66058691099284	1.21793288304503	-9.15124673179009
N	-4.02588284048735	1.62588404221857	-8.02058278506235
C	-2.61467907184473	3.56341550336469	-6.33959471904725
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C     -4.54984799710881      -0.72244652929424      -1.60740335398207
C     -5.57367477013871      -5.03699098008070      -6.98790027324877
C     -4.55956109503332       0.32648180653000     -11.47287354709207
C     -4.77366329655793       4.73674427065981      -6.07893285820895
C     -2.13125231265680      -2.18335353192614      -2.87899568348260
C     -0.78384525833523      -2.47615723427982      -2.77867796691982
C      0.17656528923472      -1.47927737453686      -2.85086140543673
C     -0.24765226317784      -0.17260814355727      -3.01676285807795
C     -1.59903378715368       0.13588916190812      -3.10915306467656
C     -2.49830538738903      -4.38883211110104      -8.01381203203248
C     -1.20561742131593      -4.89009935902569      -7.96801468321192
C     -0.62751238213501      -5.25977126176849      -6.76475540685210
C     -1.38132679516933      -5.13337102925159      -5.60875480833806
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C     -1.97308037805672       1.45377615966575     -10.15523044548253
C     -0.59509609888319       1.60441657719977     -10.18236564809462
C      0.22147783708806       0.48022933575444     -10.07599807424889
C     -0.35839849226845      -0.76724433456063      -9.96570562692711
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C     -1.78551457118912       3.56862461245137      -5.22423781342484
C     -0.43306701796614       3.85307625691801      -5.36398298234059
C      0.11277436039092       4.13214305785455      -6.60353647361462
C     -0.71670152498321       4.15944074625192      -7.72151267840752
C     -2.07046012418337       3.87169766822659      -7.58746625896156
O     -0.42068848710700      -3.78855433981320      -2.54768859591181
O     -0.86923605048096      -5.53832916783617      -4.39093364568117
O     -0.13440401185749       4.54453808745196      -8.88529894180702
O      0.05354462365741       2.78367346472661     -10.35623779354215
C     -0.53217887751004       4.02485791897248     -10.11499722685513
P      0.30546031659549      -4.71131678104682      -3.65413231290804
C      1.09701583917412      -5.94947093671023      -2.65865384213742
O      1.11497829526070      -3.92337072132794      -4.61658541409541
C      1.25997676183115      -7.24102256946118      -3.15697047104148
C      1.95425025982090      -8.18123951380460      -2.41471161181385
C      2.48810805931350      -7.83766466210323      -1.18128398511544
C      2.32864309716198      -6.55228701575236      -0.68509390839374
C      1.63666689934013      -5.60527728180298      -1.42067464382586
H     -6.18265651945807      -1.82105585246510     -10.96162808870035
H     -6.55283692114749      -3.87072169924224      -9.26210455415892
H     -3.51080664209450      -1.40458743978662      -7.77329439892322
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H     -5.72732539468178       3.81921120397127      -3.70593149506025
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H     -5.62228637818381      -0.55078199347533      -1.52295531482095
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H    -4.21536788036493       1.28692079563971     -11.85320917314089
H    -4.15711262630879      -0.45719992703130     -12.11325684070714
H    -5.64633649685615       0.30552154780495     -11.55481476797429
H    -5.85561040139330       4.66423285377994      -5.95904383084003
H    -4.57497575043003       5.32843938014824      -6.97032202790060
H    -4.36781017462234       5.27201614426951      -5.22203075868129
H    -2.84996883628789      -2.99026298965832      -2.80329350272567
H     1.22833805704759      -1.71381725344827      -2.76325616302508
H     0.48558071242900       0.62049978976024      -3.07196071647751
H    -1.89217811197795       1.17067158908586      -3.21402077264159
H    -2.92934131625513      -4.12240592837874      -8.97018657356740
H    -0.64126199279833      -4.99815990645107      -8.88464872457030
H     0.37974004585044      -5.65106069357999      -6.73002660297090
H    -3.23829504357873      -4.58023295925778      -4.71888139765980
H    -2.62392820699923       2.31267005067513     -10.24812205432290
H     1.29660085830946       0.60134443409619     -10.09180581395680
H     0.27875049870351      -1.63960355237827      -9.89885244904883
H    -2.15957985265140      -1.91431190324026      -9.86140483945326
H    -2.18778408488492       3.36498585349359      -4.24067510101485
H     0.21042822577472       3.84787120075323      -4.49403050654146
H     1.16825318885766       4.33159758775110      -6.71985737044713
H    -2.72705605536884       3.91430717077645      -8.44637289508108
H    -1.62087954168226       4.00341435364386     -10.22244016556420
H    -0.12591058207429       4.70784719299562     -10.85777699734134
H     0.84013454468241      -7.52301826345911      -4.11302108903328
H     2.07542976962971      -9.18507005678442      -2.79795016606309
H     3.02903914997598      -8.57507737507866      -0.60371807179328
H     2.74075363601934      -6.28613500435564       0.27838401576983
H     1.51168798870310      -4.60810378352986      -1.02098268046341
N    -9.04633787906001       0.22689402892668      -6.67969658945877
C    -8.62915683015487       1.03852204944056      -5.72138117048909
N    -7.30498490609791       0.97216883492220      -5.56281197021279
C    -6.75031237325136       0.06218361008645      -6.47612432882599
C    -7.91835828741701      -0.48292997277656      -7.26149923612180
O    -5.60269924147083      -0.19838370457045      -6.57831222648313
N    -9.41585985965957       1.81925549599409      -4.99983631010058
C   -10.42438470429770       0.03023670217717      -7.06705322779149
H    -9.03583527761682       2.40243069210848      -4.27384611869507
H   -10.40972413652872       1.85198287237805      -5.14638245539950
H   -10.45259221414303      -0.66868506267411      -7.89767240248090
H   -10.88308346635060       0.95904943497028      -7.40879626590677
H   -11.01572627277584      -0.39545607493895      -6.25485849295880
H    -7.99140907583108      -1.56441558902939      -7.12543401958332
H    -7.78874616487372      -0.26686866431701      -8.32453788922950
H    -6.73610816650182       1.54916118099695      -4.93507369092440
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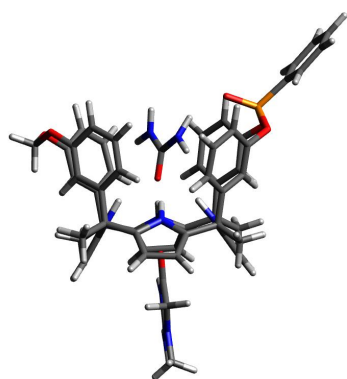
Complex **9,** $E_{tot}(Hartree)$**: -3674.991534836158**

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C    3.49639371106183        2.85418198850152       -2.59820734680897
C    4.17316099104237        4.03544997336788       -2.17977272138574
C    5.38003066781937        3.64952903776077       -1.64195808208525
N    5.43625617207934        2.29061599044845       -1.72300116551756
C    4.09955790088282        0.30203902784116       -2.50135588608074
C    6.50123914407845        4.47738328708508       -1.05917450205622
C    7.70188641333924        4.45052355241301       -1.98079300060782
C    8.11466459907866        5.37317420592534       -2.91030367996253
C    9.32483905826897        4.89982977056413       -3.47542289340721
C    9.62093645493182        3.69810144346716       -2.87749016700279
N    8.62433290328049        3.44431841244959       -1.98155365918442
C   10.80294499127801        2.77806832365538       -3.09148905129496
C   10.39426131266525        1.59004820927930       -3.93103463253223
C   10.72430927700670        1.25951902561698       -5.22394722162832
C   10.08153608386923        0.03229522025568       -5.52697695498086
C    9.37716926659195       -0.35069434427774       -4.41073184929270
N    9.58838162115509        0.59840744052272       -3.45846664285156
C    8.45375857662574       -1.52893429814161       -4.20023923830831
C    7.01925761125473       -1.04854668477651       -4.28963587946422
C    6.13933874499667       -1.02413796074160       -5.34568354809422
C    4.91136562921061       -0.50035189278565       -4.86475309235727
C    5.07709655111194       -0.22032675373132       -3.52878238408711
N    6.35902665250357       -0.54942581514954       -3.21104512831704
C    8.69305028346463       -2.23204624927917       -2.85699136824055
C    4.22395835684290       -0.45938851642672       -1.17550074126147
C    6.86637734697209        4.00226843933233        0.35063293194870
C   11.42587877215510        2.32121473213021       -1.76696556886638
C   11.90494647897663        3.55710400905275       -3.82624759200157
C    6.02484359417832        5.93136047778138       -0.91529804068164
C    2.66813383018839        0.06368536737796       -3.00366335817116
C    8.70916948714552       -2.56190164643980       -5.30681694204318
C   11.36364814279275        3.11493167352815       -0.62426476797265
C   11.98984185151066        2.70832107382355        0.54403967771765
C   12.71164884304977        1.52884932974248        0.60035574826187
C   12.80571822328165        0.75549599246821       -0.54646371320402
C   12.16417396499084        1.13921297253892       -1.71462963043088
C    5.93420706358422        3.37319359068033        1.16885518816287
C    6.26327243128461        3.01233601943803        2.46691743325036
C    7.52346150972663        3.26892036415721        2.97758717299191
C    8.43984634496200        3.92356172799229        2.17217020910580
C    8.12134446878707        4.29419320943201        0.87782818096211
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C    4.54218980860233    -1.81616533153216    -1.18404296591497
C    4.58017940026465    -2.54704609551170    -0.00349630772953
C    4.26838887516997    -1.92559278591475     1.20323265499781
C    3.91329130036545    -0.58892072631445     1.20790073232956
C    3.89998101188777     0.15063559606352     0.03124949668673
C    9.89826620140941    -2.13452534410468    -2.17709930842266
C   10.06978444156213    -2.80063858733165    -0.97009280717356
C    9.05775018100426    -3.56833531211924    -0.43052037714514
C    7.85993857466550    -3.70715440526033    -1.12640780244834
C    7.68901318555382    -3.05218332024070    -2.33662108406987
O   11.90715892654005     3.51321687641665     1.66006395744447
O    9.67689308655511     4.26901091689290     2.67076818256359
O    6.95153268588358    -4.54580610201265    -0.55841433325218
O    4.84240871233649    -3.87378540551904     0.07043605529821
C    5.60088470678698    -4.55074530415189    -0.88818913797955
P   10.88068237540378     3.20910228737990     2.87507004222503
C   11.73450757011353     3.88641565195773     4.28289190602302
O   10.43156672304232     1.80046155618551     2.94584474255767
C   10.99253874709036     4.37176238589618     5.35824840502936
C   11.63627124354851     4.78579825615960     6.51169128799510
C   13.01907265279350     4.71734363595808     6.59810880050949
C   13.76050991920194     4.23635394652550     5.52944453660424
C   13.12268682588286     3.81872212828710     4.37269823445475
H    2.49775228291047     2.79507572003027    -3.00198829963942
H    3.78824704101895     5.04175904323564    -2.22557752486189
H    6.22448433916948     1.72979160155983    -1.40971009930084
H    7.64077640790259     6.31681047210915    -3.12714059828886
H    9.93591529061464     5.42113831364612    -4.19409299754020
H    8.53102352584757     2.58651768972881    -1.45116691436735
H   11.39098058495284     1.80440203647388    -5.87300125676626
H   10.16040019942949    -0.51837972870883    -6.45027089782720
H    9.12995630994032     0.59436420752563    -2.55415711566781
H    6.33005027879715    -1.38217626771065    -6.34459030718387
H    4.00019988622623    -0.39832755812978    -5.43255143237305
H    6.77852919158329    -0.42824279320573    -2.29713353853703
H   11.56690311578657     3.91279280038851    -4.79940066912275
H   12.21580728148498     4.41909090537837    -3.23769321732632
H   12.77702567010276     2.92458063861049    -3.98238462669170
H    5.17023056979392     5.98562642365580    -0.24287614425796
H    6.82219532406546     6.54441902461260    -0.49910932854664
H    5.73448865268229     6.36202957964782    -1.87377661208967
H    2.50818673699336    -0.99890643784089    -3.17828206292013
H    1.94382814498837     0.39520739733797    -2.26091947093008
H    2.47152073191755     0.59118038426370    -3.93798369811460
H    8.55026860017207    -2.13919411007795    -6.29931459674297
H    8.04034497773977    -3.41377956156311    -5.19456980865785
H    9.73485655196948    -2.92382294590808    -5.25219069676989
H   10.83655742691178     4.05956212373188    -0.63952836257187
H   13.19298356336484     1.22013396297097     1.51871234978717
H   13.37706042671295    -0.16288303500120    -0.52468520767737
H   12.24925868518105     0.52033357241648    -2.59885055280088
H    4.93841450017672     3.16631427845495     0.80003805715844
H    5.52673918092224     2.51909133845560     3.08760693804618
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H      4.73209997289843        -2.29437308001167        -2.13473604329021
H      4.28572807712575        -2.50291766642597         2.11810868045323
H      3.64324167790670        -0.11455675302700         2.14276414429635
H      3.61366141155938         1.19324201596249         0.05758129291383
H     10.71290776166755        -1.55350938979334        -2.58531902533449
H     11.00767819170715        -2.71069696470818        -0.43792789648314
H      9.18868951601790        -4.07967063229303         0.51381828667135
H      6.78274457685016        -3.17454889407261        -2.91430379995435
H      5.41344406905247        -4.18455101548553        -1.90042919144074
H      5.27410459754706        -5.58696025098570        -0.83020331853698
H      9.91430083769629         4.43875052235485         5.29957098090579
H     11.05901138272763         5.16601941992333         7.34337092073056
H     13.51957641412641         5.04451845078611         7.49955137467603
H     14.83886707268409         4.18892838746913         5.59527803722256
H     13.71242087412003         3.45233127561410         3.54343018741877
C      8.22908664676167         0.36671271304774         0.20702644775693
O      7.87162609293798         0.66847334631264        -0.95700610993263
N      9.51758815502099         0.39094211440576         0.57421655085705
H     10.18402078751599         0.66563336637844        -0.12691478924503
H      9.79420301709012         0.59387033835673         1.52821359147699
N      7.33604311203450        -0.00362461957319         1.13274585326363
H      6.35808721419365        -0.04739691315036         0.90214973506173
H      7.62268085377049        -0.35071116691655         2.02941618884428
N      6.48414623880262         3.61057449064571        -7.00798226992602
C      5.45118073975304         3.85212187454758        -6.21657317493040
N      5.60512100627039         3.28106017868732        -5.02038421437162
C      6.83504712087433         2.60961647093424        -4.95180710560603
C      7.48136953282392         2.82186913446081        -6.30086333929612
O      7.24493134885488         2.01635672238099        -4.01633154186474
N      4.39004521547496         4.56666137562712        -6.55292720093573
C      6.64554338510271         4.11254857634850        -8.35293122731058
H      3.64862796869568         4.72226731584279        -5.89139983889255
H      4.30969707935892         5.01279532272237        -7.44997766811307
H      7.49559839806741         3.61244687118497        -8.80822685528996
H      6.83840510598799         5.18633180322346        -8.36704476187534
H      5.77349316614578         3.88809201968967        -8.96835041491305
H      7.67404071117619         1.86056654784124        -6.78255108354289
H      8.42796735201139         3.35423311229546        -6.17985910993083
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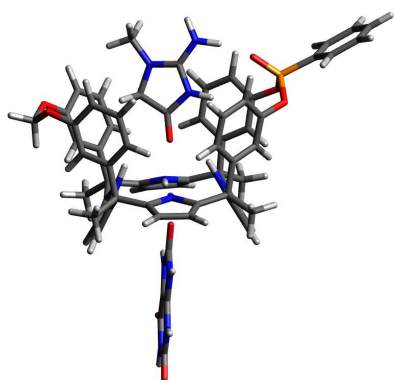
Complex **10**, $E_{tot}(Hartree)$: **-4086.538308700876**

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C	-2.49472582820050	4.96055268431980	0.92726188566272
C	-1.51762112449673	4.35443129831612	1.67587096495999
N	-1.56193050646132	3.01914082365466	1.39069678956826
C	-2.85271758484275	1.35352084807987	0.02586466594038
C	-0.63590161893343	4.91237031276678	2.76553471506750
C	0.79984226656983	4.45194271249830	2.64163787156348
C	1.88291120270416	5.05883983290534	2.05700221588810
C	3.00968794957728	4.22732718477651	2.27241646299675
C	2.58996425098441	3.13099247235116	2.98268055603582
N	1.24900500303448	3.28463732418138	3.18909611678072
C	3.36536239131152	1.96382113246714	3.55104684849716
C	3.26407060008788	0.72604228743839	2.68982021516785
C	4.18678790423268	-0.26141713204093	2.44186794900913
C	3.52017563494024	-1.30491299598704	1.74682128338189
C	2.20964277452372	-0.92429622414620	1.58926405835978
N	2.07433694524145	0.29961402949449	2.17603543206319
C	1.02775137417014	-1.67979435622484	1.03106127572222
C	0.14191213594482	-0.79612242763778	0.18146678150960
C	0.08984815170477	-0.61830787564524	-1.17780607123181
C	-1.00972694144732	0.23096901375922	-1.45913813651158
C	-1.60563233433391	0.55276629615273	-0.26568661007491
N	-0.87940180161681	-0.06259152458513	0.71490796213624
C	0.18112622983690	-2.29984734434272	2.15844588792487
C	-3.71408993919057	0.65482833406040	1.09754047435166
C	-1.19068044723186	4.53298666083748	4.14802408560082
C	2.86452412462056	1.65389274676582	4.97379627816207
C	4.84520684556034	2.35717508930777	3.68002734331506
C	-0.67197955782068	6.44764966598207	2.68562901847555
C	-3.71626351874874	1.41257519848989	-1.24458755112666
C	1.55145340444151	-2.83924317082926	0.16893616842254
C	2.56839363186214	2.70266494401256	5.84506159868821
C	2.19481520701560	2.44281646412510	7.15276960171639
C	2.10744024192619	1.14488303371718	7.63690659594982
C	2.40273876623470	0.10476780414150	6.77022252170667
C	2.77031966779006	0.35212408318258	5.45566807776979
C	-2.46365888536947	3.99875309028504	4.32222849689501
C	-2.97266905711504	3.77570547563535	5.59483384164527
C	-2.22461266655520	4.06705586582944	6.72361672584470
C	-0.94935430588045	4.58074126827348	6.54563392680001
C	-0.43234560260632	4.81425744767817	5.28444468978609

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C   -3.78612641970648      -0.73947529154840       1.13009654350194
C   -4.65148808397416      -1.39233569025920       2.00066824428156
C   -5.47498843845572      -0.64655765605976       2.84242950186281
C   -5.41150495105693       0.73548593336550       2.80531399073022
C   -4.52748291174287       1.38866626555296       1.95573138241345
C    0.62944288589228      -2.38404935665278       3.46991792162573
C   -0.14473156203367      -3.02303757853218       4.43058444277412
C   -1.37732816147850      -3.56438729230460       4.10902295196197
C   -1.83814198059184      -3.48090899146474       2.79619744933059
C   -1.05675061642107      -2.85809792755372       1.83313758990463
O    1.95778791633054       3.52104706251151       7.98864959334594
O   -0.18097402659229       4.93197843944725       7.64166201704211
O   -3.02167745309428      -4.10019264466031       2.54332621774017
O   -4.81773693020129      -2.73580558259490       2.07887164414230
C   -3.90763708750941      -3.66022112896851       1.56222859011923
P    0.51063248686238       3.85192485334176       8.61057391994935
C    0.90198424767147       4.81875079882762      10.04462004023410
O   -0.31366182970636       2.62005456211431       8.77892971400642
C    0.07020490082665       5.86940703699486      10.42927205917024
C    0.34943351230162       6.57834899015600      11.58552962566914
C    1.45089280086806       6.24245831072826      12.35903322330671
C    2.27914789584383       5.19675090090863      11.97767072358955
C    2.00881090450651       4.48256035114605      10.82281322902476
H   -3.94647997778250       4.09892278824090      -0.53417568649784
H   -2.75994659195883       6.00451561603987       0.94062668132186
H   -0.76884109603433       2.41033126021453       1.51794582117615
H    1.88241338827053       6.00705362049414       1.54350973655803
H    4.01975947088569       4.43597307642054       1.95895604102516
H    0.67664724300353       2.63263530479500       3.70115066277821
H    5.21932352197100      -0.26683186981640       2.75162681936030
H    3.95930993149079      -2.23832405098447       1.43323051039039
H    1.32905535488319       0.93562578682498       1.93938607183950
H    0.74265653496469      -1.07433917678865      -1.90447350356762
H   -1.33502527299117       0.54368553790122      -2.43803784167768
H   -1.11279202478847      -0.05564123713414       1.69405955251195
H    5.27970220935840       2.57161986644344       2.70443656116898
H    4.95728201080523       3.23830793527673       4.30885217931120
H    5.41760857084385       1.55019609234237       4.13424624359520
H   -1.67678823086369       6.81779915503437       2.88280411727060
H   -0.00458889500971       6.88716046822502       3.42457983368143
H   -0.36802826575708       6.79620235722226       1.69934657268879
H   -3.96206256464196       0.40862682097623      -1.58693002610034
H   -4.65214010159868       1.93265825802521      -1.04496121672469
H   -3.20056113930479       1.93945617305724      -2.04674030179082
H    2.19165415054279      -2.47226271863245      -0.63212337991362
H    0.72597962274256      -3.38933042090870      -0.27871371178650
H    2.12862452951246      -3.53716969111974       0.77313307679053
H    2.65118640867702       3.72939192913653       5.51066968701531
H    1.84271916573889       0.95229138748008       8.66732903616359
H    2.35648144566658      -0.91497914620287       7.13030120635698
H    3.00916924012471      -0.47968373216655       4.80797489485140
H   -3.07978552111794       3.78607372424404       3.46006501993036
H   -3.98007374224843       3.39449178193527       5.70649457284693
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H    -3.17548021414001    -1.29517157976014     0.43215682330302
H    -6.18361208217042    -1.15796854803725     3.48222119549553
H    -6.07135441026969     1.31645048390725     3.43790180404526
H    -4.50671686236207     2.46999201403551     1.92773232095141
H     1.59194611268082    -1.97484589863459     3.74030853451520
H     0.22599869180589    -3.11029077730183     5.44458899768623
H    -1.97186528341050    -4.08370088832606     4.85002252152798
H    -1.38062124377015    -2.81602081024566     0.80040950090103
H    -3.40120187565929    -3.28912420489880     0.66835683222891
H    -4.49632475021023    -4.53249553029286     1.28753890824684
H    -0.78341621514176     6.15256219413450     9.82865633047387
H    -0.28982349659634     7.39984888275057    11.87932065261426
H     1.66819405228037     6.80050041998567    13.26004820837496
H     3.14281619616358     4.94074881195398    12.57613638406217
H     2.67231343419312     3.68065897747046    10.52833265928028
N    -2.87689083512826    -0.18437155634015     6.07706787500295
C    -2.02136499181894     0.51075926457552     6.80739061682785
N    -1.02446882771997     0.99455691547078     6.02578419662945
C    -1.22418001142715     0.65312198757007     4.70708539867696
C    -2.48512613304603    -0.16245386514462     4.68053581362526
O    -0.52735688440495     0.95754785910771     3.78157272485812
N    -2.07384840717174     0.72792594238292     8.09556037129669
C    -4.04413677148756    -0.87405150118506     6.57631512066531
H    -1.41712368660101     1.41263693035712     8.51192463371339
H    -2.82594942349696     0.36148844893960     8.65343212067431
H    -4.57268482344495    -1.30667294612176     5.73138212757041
H    -4.72861407950951    -0.19097382027171     7.08081087590897
H    -3.77053901222637    -1.68556249865372     7.25149878811413
H    -2.28773978592788    -1.16515408395112     4.29375239343207
H    -3.24000186533627     0.32214052630982     4.05540716295195
H    -0.23602483347353     1.52351623320009     6.38257633788720
N     2.57179778432937     4.11015798224963    -4.75592835568810
C     3.70614014725941     3.34717265478284    -4.57849075996661
O     4.59241637981683     3.26348541687963    -5.38670036519236
N     3.75019922811054     2.66765271868692    -3.36771421901845
C     2.72607626150164     2.76895092435534    -2.48345253192088
N     2.59982611669492     2.19123287262557    -1.25923001463236
C     1.39352604899501     2.58453546942372    -0.67716170939683
O     0.99695651484659     2.25246994395383     0.41808840745236
N     0.81308120977735     3.39889622820280    -1.59208473826849
C     1.62587832059041     3.52248189625589    -2.70965396265781
C     1.46724457613769     4.28385295878825    -3.90716190390825
O     0.53862689547042     4.99637458372754    -4.20171793957305
H     2.53717778683424     4.61265173751471    -5.63298141949728
H     4.56342556990254     2.09688918904771    -3.20348235027191
H     3.23741305310877     1.56550013424002    -0.79399025316013
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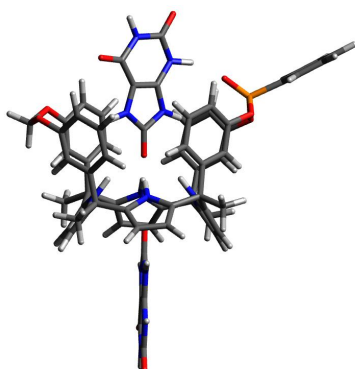
Complex **11a,** $E_{tot}(Hartree)$**: -4327.202864607931**

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O	-3.93205539505595	11.39668502863702	3.66863967989080
N	-4.41868606664815	9.17672937481934	3.71727115581181
C	-5.12452751565263	8.19849905789349	4.32888995137382
N	-5.11047008066169	6.86549104294501	4.05643782528614
C	-5.97066827647017	6.20939189367652	4.91272328139765
O	-6.17152482815720	4.99085941941036	4.93660820526109
N	-6.50842842964228	7.16381181545731	5.69264780435684
C	-6.00536881332183	8.40673384531529	5.33722860295583
C	-6.27336643378938	9.72207321785882	5.82816040724481
O	-7.02502291150498	10.04363330327707	6.71864281896600
H	-5.64674022524193	11.62888758975626	5.41047274520263
H	-3.58024288328967	8.93242327774021	3.18491581397426
H	-4.56179260366382	6.40386872082631	3.34565123662527
H	-7.20134387291468	7.00338178866830	6.40977108144279
C	-8.52472873966119	2.71233852739107	2.70018200290471
C	-8.64987987316526	1.66065632167684	1.82419275781292
C	-7.34460315500585	1.30335353741551	1.39738009306436
C	-6.45960389333959	2.14676307644928	2.02684458221630
N	-7.19689165038580	2.99034801084620	2.79890183747335
C	-9.57474180552778	3.43774717704958	3.51002696063954
C	-4.95631823806221	2.24274930691194	1.92734456456443
C	-4.29529067913966	1.82504180231229	3.21992255070257
C	-3.62968178368540	0.67270245767119	3.55520510188530
C	-3.16164073173183	0.82026497518515	4.88544126066111
C	-3.55462870221528	2.05951609421793	5.32376561245462
N	-4.23033895658612	2.65055529184807	4.30127939387062
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C	-4.52282344741728	2.55948523861743	7.54431687966767
C	-4.66981042045758	1.75078739048484	8.64762890788981
C	-6.01344290372430	1.86424207047723	9.09062643429268
C	-6.65541021482929	2.74108353924367	8.24625808758013
N	-5.73753388433792	3.14791909529374	7.32796559145755
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C	-8.85232077321760	2.84185571454144	7.06776649202108
C	-9.86916008921308	1.92937293615733	6.92576782815743
C	-10.30805365885429	1.98385476929995	5.57805341871167
C	-9.54599532299387	2.92804850211408	4.93569824989159
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C    -2.09955222720657      2.16059457022413      7.33161192537958
C    -4.47136482912623      1.32020273616269      0.79965113787430
C   -10.95364408231444      3.14795050857930      2.90152703638332
C    -8.76471989642331      2.73118826510959      9.54154187892802
C    -2.11291608090654      4.56312183862560      5.36794311878341
C    -1.74948867971516      5.87550084208634      5.13601641916981
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C    -3.16526828602651      6.60132564130546      6.89835830677928
C    -3.52967494651529      5.28407655477365      7.14999839448374
C    -5.35978227963085      4.52130186125063      0.84281270727385
C    -4.92128921690168      5.77866286748001      0.45311272883900
C    -3.63847107256558      6.21123010402156      0.75118651807015
C    -2.79875033223199      5.34443563099485      1.43555756319730
C    -3.22532241025744      4.08963220728649      1.83195160094495
C    -9.99268311349737      5.71287964899488      4.50909256361095
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C    -8.14585714249246      7.58849862090115      8.71841305268894
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C    -9.17820582861628      5.53811300766463      7.98454166278887
O    -0.79822265626594      6.12006418268598      4.15868739404172
O    -1.48885191907705      5.69422155312136      1.70530153089218
O   -10.29887197331094      7.68227898775489      7.81430263801911
O   -10.37869654444015      7.89535596088498      5.52523061763815
C   -11.03615210700287      7.42536476082713      6.66293245900993
P    -1.10305118757444      6.85238786923399      2.76049633226361
C     0.53071221195747      7.31157084999780      2.22063204530026
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C     2.77826268319450      8.01778762437194      2.69870884357006
C     1.53520607748044      7.59644174837214      3.14246668183774
H    -9.56977163388979      1.20068113622592      1.50270278830513
H    -7.10157047582005      0.53173254484730      0.68470266294698
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H    -3.47478033805288     -0.18122423945587      2.91595514819367
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H    -1.98237729847091      7.94039804628896      5.69845125991352
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H    -4.22310249738242      5.07827100063168      7.95223957294520
H    -6.36137993301447      4.20367639443987      0.58649065613421
H    -5.58652124977833      6.43256783716641     -0.09541209647816
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H    -7.91867244708971      7.51432902361215      1.83321745777776
H    -8.19455688497089      5.07917339546843      1.71493211413708
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H   -11.31745927966378      6.37294191161702      6.58033607078449
H   -11.94384430343105      8.01667704076305      6.77268633547497
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H     2.21189493571582      7.98860623347330     -0.63743466767070
H     3.99427777265290      8.48758435832936      0.99829068440685
H     3.55868190125532      8.23101545109673      3.41631213075585
H     1.36000389024025      7.48192877116850      4.20326210528517
N    -7.73425668184137     -4.12790484399702      5.33823991933740
C    -7.30982096278087     -4.07098546364012      6.64562829771076
O    -7.26549107526626     -5.02718939426017      7.37925968334392
N    -6.93000928366041     -2.80513334221754      7.05963099815635
C    -6.99239286226585     -1.74681951895856      6.20756195997642
N    -6.66167139160933     -0.45580692852552      6.44407129648491
C    -6.87785511700837      0.30396780705364      5.28363650333947
O    -6.67911131295122      1.48579812545314      5.17119710465692
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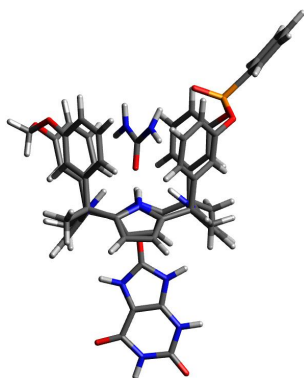
Complex **12a**, $E_{tot}(Hartree)$**: -3915.642021536771**

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C	2.30341958665494	13.94921127152987	2.97890096447559
C	2.58788049863202	12.85025983892869	3.75229000903402
N	1.42043296378921	12.17032492925284	3.92391603346492
C	-1.02523892509795	12.28254446735720	3.33248039586332
C	3.89628634278096	12.39593131431636	4.35805210548607
C	4.46923344259649	11.22478537234384	3.59232011054848
C	5.54925333794654	11.15230304629466	2.74411527483087
C	5.67566183831928	9.79790468091091	2.33356251227330
C	4.66892335708815	9.08413744110876	2.94328603576126
N	3.96423195006276	9.96662390934488	3.70212586149662
C	4.37022463867557	7.60294866872714	2.91222607728403
C	3.05235612739248	7.29934862977976	2.23500715361051
C	2.79609196775029	6.63502606196434	1.05996876747896
C	1.38957954370925	6.54165997252011	0.91885216614617
C	0.82516230857236	7.15117197252546	2.01177819392990
N	1.84600992796256	7.59123279181577	2.79714878527572
C	-0.62641852363577	7.37111167103506	2.37651374698920
C	-1.01490297687719	8.80962253137586	2.11048433326180
C	-1.73628341053452	9.37380232175123	1.08569373494580
C	-1.84485057534432	10.76320923582320	1.35858124152109
C	-1.18498106270313	11.00408751621651	2.54212200565177
N	-0.69807194400093	9.81143513734924	2.97395036216999
C	-0.88336463320617	7.00750072416993	3.84697167427644
C	-1.46263167585024	12.08955794536414	4.79380985184507
C	3.73646364954233	12.03683849025679	5.84230020988522
C	4.38786006639055	7.00818765857105	4.32846756932132
C	5.49171005246147	6.90163210024924	2.13235809132341
C	4.89873388736608	13.55764640223371	4.29737096936953
C	-1.95586181835289	13.34520053221721	2.72998692217092
C	-1.50265959880509	6.45052638792332	1.51770527767063
C	5.11944483815623	7.59639708803732	5.35678193298509
C	5.14626459572387	7.01882879167803	6.61618443868466
C	4.47686395584310	5.83757799323238	6.88200929328939
C	3.77849508398883	5.22970633002463	5.84903640224882
C	3.72411514579506	5.80978844337476	4.59099151038229
C	2.76568553781751	12.64242541198773	6.63413384968654
C	2.67196472029365	12.35191203574704	7.98649387063370
C	3.54123967543482	11.45500140532913	8.58422924172594
C	4.52732473587249	10.87992915813523	7.80191422549483
C	4.63327033309386	11.16276712156888	6.45237607107865

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C   -2.34482974909068     11.81547393930096      7.43784918601935
C   -1.41150156293269     12.78221433333582      7.10274836978843
C   -0.96108461199425     12.91571286836718      5.79650229683122
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C   -0.39895625900532      5.71090000433050      5.81245848025857
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C   -2.12687047075003      7.36470122062333      5.89330655191978
C   -1.90046023836461      7.64752294451610      4.55382691401207
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O    5.47203707219510     10.05047244308743      8.37732298580240
O   -3.05373774798453      7.97459886488640      6.68117922710253
O   -3.83427727939917     10.12723393973532      6.83089292069731
C   -3.99323920490789      8.89141824563982      6.20915169575609
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C    6.35873239366914      8.28890962977864     10.12641050008953
O    3.78216544468609      8.19075695278768      9.05537574316409
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C    7.38717800062326      9.10549462813230     12.14221966862010
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H    0.37449148899426     14.64041016195927      2.10060719037110
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H    1.34001711496158     11.28425336536531      4.40550599214481
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H    3.25698455144446      4.29990324481248      6.03427352862439
H    3.16426965757872      5.32541301876341      3.80158254308859
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H     -2.68971157258173      11.69910151546469       8.45690849998554
H     -1.02181272844919      13.43653783666426       7.87257342337550
H     -0.22981343311711      13.67650987175317       5.55575475067235
H      0.61675664223244       5.47446949733043       3.94201801097986
H      0.18402500696148       4.94405896852703       6.30586639753082
H     -1.54205361089477       6.17105613348957       7.57426494550064
H     -2.49731087727152       8.37719761318786       4.02829333994464
H     -3.99129812005710       8.96977372812112       5.11969449659725
H     -4.97652973740204       8.54594479268394       6.52744500686981
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H      7.56241250534664       9.91079522840173      12.84284193885492
H      8.59924393036704       7.69891824039015      13.21332924366947
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C      1.26673053940906       9.13270500510921       6.31057145324054
O      1.30437198268778       9.42498213558118       5.09338891760892
N      1.91418661725035       8.06684332649970       6.79816821961701
H      2.42769038853305       7.50276006014738       6.14337743059884
H      2.25203428252651       8.03755970817591       7.75094133541350
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H      0.07504956003754      10.69261017553651       6.85134313321689
H      0.40824385725356       9.58120769992026       8.12101638771456
N      2.53283842083183      11.95721083428907      -3.65924310742124
C      3.87708499775191      11.99826632839721      -3.37134069312002
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N      4.18391935798659      11.63695837993168      -2.07143204142347
C      3.20255451362968      11.28441599944775      -1.19857208750378
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O      1.84094630985749      10.29264182201800       1.76371171014118
N      1.19670195706736      10.85776530937071      -0.39507056407346
C      1.88617756531547      11.25982845962450      -1.52955851139353
C      1.44317901692176      11.60832377276040      -2.83686346536279
O      0.30992984411527      11.62773484783252      -3.25952800021587
H      2.29466840426684      12.21806417015011      -4.60555892882328
H      5.15795856473306      11.63928894931498      -1.81746728652311
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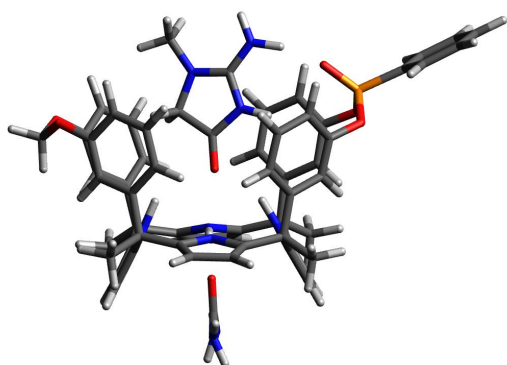
Complex **13**, $E_{tot}(Hartree)$**: -3674.985515649129**

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C   -2.25610100644486      4.16458837876425     -1.50773767833583
C   -1.25309301300930      3.39271010722852     -0.97861500987790
N   -1.07500152867565      2.32427729637273     -1.81278726354958
C   -2.04803219079547      1.30097159407957     -3.89719022380431
C   -0.54996024318088      3.48885487328977      0.35321875126823
C    0.93218539043735      3.20243123757813      0.25117110958869
C    1.99993076087801      4.05637156972398      0.13376655721004
C    3.17981472901341      3.27314844556429      0.14551957591606
C    2.80600908989766      1.95787875235551      0.26768954751365
N    1.44283555670849      1.93881959047256      0.32402316036095
C    3.63825323548933      0.70392816733499      0.41029717999776
C    3.77040061740336     -0.05948171271557     -0.88667040996012
C    4.81786554326980     -0.80213251781736     -1.37516705123501
C    4.35084259699487     -1.49558447654114     -2.52253366840154
C    3.03279956048374     -1.15373638262485     -2.70254993593952
N    2.69711745852143     -0.29752574470256     -1.69550273363127
C    2.01072548609394     -1.66807870737649     -3.68762208917374
C    1.12226271274863     -0.56231530255026     -4.21331226280377
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C    0.05219985171477      0.99989352435720     -5.42974974075850
C   -0.69958927808035      0.75872864349454     -4.30782286259144
N   -0.02302852184922     -0.17568387388408     -3.57553450652185
C    1.13295359282440     -2.75876639370319     -3.04609428106046
C   -2.94681854438930      0.17378336466823     -3.34666513965253
C   -1.19895811610096      2.52413636013066      1.36052621312765
C    3.02445980862977     -0.20709816557987      1.49014814592724
C    5.04133728411696      1.09287666442230      0.90219787717293
C   -0.74461606460133      4.91089176250563      0.90474115714719
C   -2.76045514087079      1.85261744301960     -5.14309699312695
C    2.75356720434028     -2.31591841893948     -4.86646455282601
C    2.52348685461816      0.34962056287498      2.66717823490213
C    2.04431075807670     -0.46621778648351      3.67836975101343
C    2.05041424957989     -1.84901329878504      3.55991484874474
C    2.54712094359912     -2.39982671426181      2.38953183543649
C    3.02184640908437     -1.59278051372684      1.36632878360690
C   -2.40997269970432      1.88669691460997      1.10879451117002
C   -3.02207010043540      1.11035528144938      2.08406565297812
C   -2.43888165300348      0.93648331613906      3.32814220253031
C   -1.22027384001931      1.55251681009891      3.56660199682737
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C    -4.72917930869923       -1.83433193195902       -2.55300281539506
C    -4.82087072902116       -0.56020498881921       -2.02189136362802
C    -3.92977565366598        0.43640825273761       -2.39747265369278
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C    -0.80629658432369       -4.20558043252605       -3.21533916769671
C    -0.00540403178228       -3.19447395886171       -3.72816104314440
O     1.60774683944655        0.13425346982957        4.84758638421533
O    -0.61760775869232        1.44799819605972        4.80856024796724
O    -1.89930593940849       -4.71575230664218       -3.84390001970380
O    -3.76518634968039       -3.37598555652234       -3.99069694838453
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C     0.20839520869882        0.39117712388789        7.08093093911274
O    -0.62790707538672       -1.13077562249044        4.86645832327033
C    -0.76696166385322        1.13708196395300        7.74143454647753
C    -0.67953374020514        1.32101623571708        9.11099600664048
C     0.37236005439868        0.76271445107408        9.82213679047836
C     1.33919744453376        0.01356762446970        9.16737739760405
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H     1.94996557609098        5.13071626162303        0.06586783530161
H     4.18972160990886        3.64697188374440        0.10021032797786
H     0.88792233040405        1.09983798599188        0.39033477330885
H     5.80375889027685       -0.87813678815749       -0.94593136432330
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H     1.93184534255565        0.35720856524149       -1.77853521065269
H     1.98101247420720        0.11096947056595       -6.10757447168434
H    -0.19725062699579        1.67946094533111       -6.22827881802311
H    -0.36166233959387       -0.59133456693274       -2.72386261074588
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H     4.97962348706699        1.66139888697473        1.82919745726246
H     5.64673249698757        0.20779085293080        1.09362531407214
H    -1.80195341454846        5.12485348079822        1.05630180050606
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H    -0.34373402255511        5.64971144650145        0.21196009573270
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H	2.16043443466604	-0.41818896472312	9.72265297057629
H	2.03069680548472	-0.74649319844273	7.29621556691149
N	-2.52550112758961	-2.67011189920693	0.90552988284379
C	-1.83685463542322	-2.30362746429523	1.97410219768421
N	-0.82955349577325	-1.46985767986412	1.61847774396970
C	-0.85480454312233	-1.21965470716935	0.26387019756833
C	-1.99688709922034	-2.02780744549367	-0.28270143622896
O	-0.11508542991756	-0.49652525756317	-0.33884415029128
N	-2.05017106848670	-2.67082103434749	3.21116113227201
C	-3.62929659602390	-3.60237115549906	0.90077892464831
H	-1.52861580119805	-2.19849955491904	3.97104397876195
H	-2.81576558338297	-3.28027974571244	3.44265975149546
H	-3.99884165240239	-3.69342654269909	-0.11675388210043
H	-4.45370424747330	-3.25025368958037	1.52232507846654
H	-3.31465052117378	-4.59292573796095	1.23178081474106
H	-1.64109108035178	-2.75300419374673	-1.01847366117362
H	-2.73388536070015	-1.37320437078322	-0.75714900432258
H	-0.15842993873627	-1.08152571277618	2.27289600300259
C	2.19871045483087	2.96691977724805	-3.26349138021613
O	1.59317556790610	2.12005006432610	-2.62393747294441
N	3.48008258172887	2.77604860820490	-3.67957358980289
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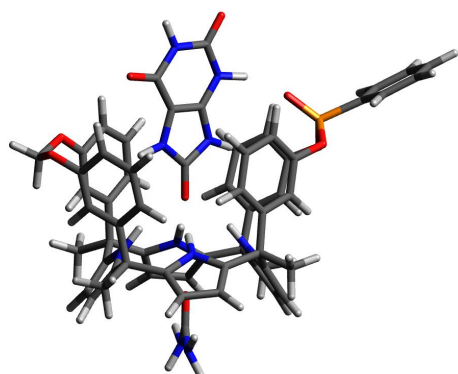
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N	2.81867872968329	-0.44285788667999	-10.40026425477414
C	1.51244283512759	-0.10066923466242	-10.32717964927665
N	0.56552261744392	-0.60754233025290	-9.49186834074055
C	-0.64206990402377	0.01103311404486	-9.73532261699318
O	-1.69807188893766	-0.21245740963528	-9.13532395332536
N	-0.41279448884367	0.88904887880777	-10.72727871435141
C	0.91619476909356	0.82421041816153	-11.11907891107883
C	1.64983754504161	1.51240865480381	-12.13442221330481
O	1.24831710018428	2.35627739778340	-12.90116769560207
H	3.57235237398738	1.51604762314547	-12.84472023757544
H	3.25675262156002	-0.92643869243633	-9.61185319895949
H	0.69388309321381	-1.33043585920226	-8.79853066830900
H	-1.11884709634349	1.47662315359106	-11.14657363436392
C	-4.41950386708838	-2.98734097708783	-9.71887083501247
C	-5.05816239706297	-4.11467375899443	-9.25807353120020
C	-4.44159813390717	-4.48304464501169	-8.03444554339691
C	-3.44659349493765	-3.56867683911950	-7.78158225162432
N	-3.44983360378643	-2.68454783360629	-8.81534899899704
C	-4.68317852790573	-2.13775063421740	-10.94032353505947
C	-2.44415750414491	-3.50072203035492	-6.65463201695448
C	-2.61549759102323	-2.25524534554120	-5.81699972379409
C	-3.11394670059268	-2.09187994018498	-4.54932344501696
C	-2.96906108273055	-0.72507991022381	-4.20349631291591
C	-2.38297931227395	-0.09220246723490	-5.27029296088588
N	-2.17073129896426	-1.03488496110160	-6.22823497892010
C	-1.96776548308721	1.34790534135029	-5.47089243521943
C	-3.03331263363647	2.09623075812994	-6.23625650589940
C	-3.92652679533878	3.04805212070009	-5.80592335279400
C	-4.75360761276548	3.38472875037764	-6.90764564974746
C	-4.34290821159546	2.63085773137789	-7.98124332603567
N	-3.29880564775101	1.87015442037761	-7.55188665873645
C	-4.82250583357652	2.62950536804599	-9.41523315163649
C	-5.39716026820159	1.29095778316813	-9.81469116011090
C	-6.68828770782481	0.90588778599878	-10.07733693775877
C	-6.65224634793120	-0.43942797801245	-10.52475893594649
C	-5.33829106289535	-0.83856513063461	-10.52365894257426
N	-4.60353296962857	0.22080206598760	-10.08985321456427
C	-3.68013392041533	3.02580445908413	-10.36594938369474
C	-3.39561598976582	-1.84302894956524	-11.72720573457587

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C    -1.01124895483414      -3.57603370581088      -7.19802157755924
C    -0.59519220162112       1.39141606206628      -6.15800059821524
C    -1.79507340580557       2.01771223276552      -4.09935269644873
C    -2.63651059114377      -4.73139285161602      -5.75673012970172
C    -5.62404780329865      -2.90410477418230     -11.87951591413237
C    -5.91174786539492       3.70156267908102      -9.56665454959653
C     0.40628947452062       0.53673107542941      -5.69646324814106
C     1.67613079304406       0.58641367954992      -6.23700832396309
C     1.99892660238263       1.46888087221898      -7.25581936743357
C     1.00498623856368       2.31470694413686      -7.71763862452279
C    -0.27344601827893       2.28467408951797      -7.17311890914485
C    -0.72321637728871      -4.19368837012763      -8.41140939466316
C     0.58674777336703      -4.31516941686198      -8.85201918832147
C     1.64164529939871      -3.82594253552310      -8.09673224133062
C     1.35189750658475      -3.22477927370091      -6.88025141823872
C     0.04928006784486      -3.09505445319130      -6.43232823652749
C    -3.37798731042598      -0.75424731324023     -12.60135823895693
C    -2.24387803203511      -0.43997560438536     -13.33417514432332
C    -1.10655085116038      -1.23748393418655     -13.21876457792630
C    -1.13448321373192      -2.33581873747734     -12.38261105307108
C    -2.26856643745979      -2.64746742091816     -11.64068543762485
C    -2.64076977787028       3.84269823391651      -9.93170254974335
C    -1.64752825837544       4.24101139914743     -10.81543574559375
C    -1.66959006732270       3.83890801935915     -12.14029671119212
C    -2.72964572096709       3.06129567450258     -12.59292954046609
C    -3.72350183294968       2.65291161605276     -11.71009140529259
O     2.64449240145810      -0.23621365040737      -5.68320858398262
O     2.36732848351700      -2.77910109313569      -6.05391665183110
O    -2.75457484560099       2.79955879055989     -13.93027123801872
O    -2.12943283266475       0.60447705119928     -14.19455682844455
C    -3.13522707907268       1.54896096867568     -14.40224710867448
P     3.29153082562514      -1.50785375707175      -6.42070637404995
C     4.73796058120077      -1.80655658435434      -5.42467430975629
O     3.46231750326699      -1.34093062262701      -7.88393216825984
C     5.28202508659942      -3.08904737000504      -5.38726464929031
C     6.44282511599777      -3.32613764636798      -4.67115718021493
C     7.06496932264839      -2.28860072045944      -3.99202870410120
C     6.52828338298961      -1.01089802043095      -4.03190860488320
C     5.36780811563526      -0.76512497669954      -4.74775160018995
H    -5.86691523605342      -4.63837364452700      -9.74166873309871
H    -4.69636521228469      -5.33802755359006      -7.42874359668121
H    -2.84748725469594      -1.87785173509056      -8.88649535994206
H    -3.52225327433159      -2.86622863699281      -3.92119320554396
H    -3.25556893583185      -0.27337450184526      -3.26803736595916
H    -1.82760533976617      -0.82099944934962      -7.15339230593130
H    -3.97891680887791       3.47745616627317      -4.81856768842832
H    -5.54069617510663       4.12046201093612      -6.90876100242516
H    -2.84096502514000       1.15947404381909      -8.10232510452341
H    -7.56670735926716       1.52214535487926      -9.98059478843360
H    -7.50139034386542      -1.03160609820868     -10.82494130473316
H    -3.60369664965827       0.19601976292905      -9.96134674995190
H    -2.72458301405123       2.00059692324858      -3.53125405612452
H    -1.03566383716929       1.50219039391915      -3.51360574611855
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H    -1.48657556496003       3.05549732611574      -4.21920196449762
H    -2.48627687011252      -5.64721321963304      -6.32676786724233
H    -1.92188664538137      -4.72076353597628      -4.93523697097846
H    -3.64175441794519      -4.74951861789264      -5.33646140281543
H    -5.83408327117777      -2.31962151264126     -12.77364284840030
H    -5.16690582274126      -3.84385221357285     -12.18655511144240
H    -6.57349789120306      -3.12783587143253     -11.39362902933691
H    -6.75592420216191       3.49825897095311      -8.90729205969131
H    -6.27521095947675       3.72982286183681     -10.59260861980682
H    -5.51304752993363       4.68591454621536      -9.32363421251539
H     0.20302820689609      -0.16627548997712      -4.89759179289241
H     2.99842096421706       1.50108599354754      -7.66838333974325
H     1.22584122987006       3.01364115407130      -8.51397840444388
H    -1.01843910409287       2.96873427768586      -7.55176823357198
H    -1.52895032070668      -4.60352308967790      -9.00541698158290
H     0.79170628755965      -4.80217384538784      -9.79646629690583
H     2.66287562624182      -3.92929906836914      -8.43621271743391
H    -0.13873682194796      -2.64040640248389      -5.46798209057196
H    -4.27593989685566      -0.15802028395640     -12.67486295628433
H    -0.22222733048410      -0.98548140555961     -13.78978647391112
H    -0.25728181223789      -2.96557210717004     -12.30442499938107
H    -2.26184384311738      -3.51452787876974     -10.99545637313450
H    -2.61491149790552       4.18143206707650      -8.90380851557449
H    -0.83534081238724       4.86511763413676     -10.46516863543484
H    -0.88644631524230       4.12377685206148     -12.82837754449880
H    -4.56605851706992       2.06775531366370     -12.05849539543042
H    -4.09788501127405       1.22845773221363     -13.99776639339637
H    -3.24092364335832       1.67555216374583     -15.47888003882117
H     4.80034974980048      -3.90823165245057      -5.90452870235698
H     6.85860951501395      -4.32383603151622      -4.63840950496144
H     7.96917755314929      -2.47711637385759      -3.42871185377862
H     7.00995808687234      -0.20214275861995      -3.49966399118115
H     4.95581086763362       0.23410533638093      -4.76616589097248
C    -5.89776501994625      -0.72392892559639      -6.70229743819473
O    -4.84331392878606      -0.58486768410151      -7.28349003701757
N    -6.53241493148176       0.30925627429414      -6.05643261658535
H    -5.97385414978727       1.14616402049180      -5.98083575878065
H    -7.06552495097777       0.08718081848425      -5.23345989134542
N    -6.55869111164704      -1.92689398378146      -6.63420617315120
H    -6.17589805826350      -2.63520903139388      -7.24335360963019
H    -7.56370125987732      -1.90235347531543      -6.60989191189518
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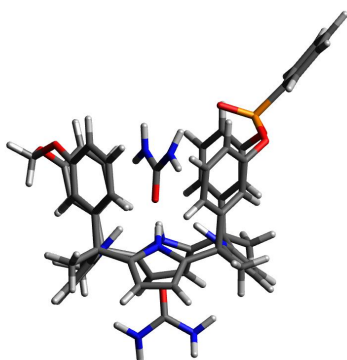
Complex **15**, $E_{tot}(Hartree)$: **-3504.074228100304**

C	-1.71985160195702	2.11376615527921	-3.11307598344465
C	-1.73145029674827	3.43349934412177	-3.49077406115946
C	-1.18047195486633	4.18722363819756	-2.42635300759760
C	-0.84695002042326	3.30713109716585	-1.42724868713435
N	-1.18862121213204	2.06158719511056	-1.86014950768059
C	-2.27017139755734	0.89399298416835	-3.81497517649123
C	-0.22776625125381	3.56345372250422	-0.07296303645203
C	1.22445625708838	3.14803556405041	-0.05728961687156
C	2.36762429825468	3.90615713480688	-0.00822975472622
C	3.46764647342799	3.01172375701906	0.03534003963209
C	2.96341675353023	1.73210413654053	0.01297493384170
N	1.60770714046037	1.84232044769607	-0.03286172356508
C	3.68096633174136	0.40648467252510	0.10600663749433
C	3.51302742587761	-0.42333523355576	-1.14634240336663
C	4.44249622554949	-0.81307528602651	-2.07956171774636
C	3.78998543626995	-1.66580285597385	-3.00318544758855
C	2.48011068684973	-1.77468445921861	-2.60785070066247
N	2.33747899295781	-1.02379946502902	-1.48116168219987
C	1.32818231837177	-2.53802135159284	-3.22271479024926
C	0.42969025207759	-1.59458963594478	-3.98843508067059
C	0.25144849327939	-1.41291980797999	-5.33843537104785
C	-0.76245895105874	-0.43270889608873	-5.50312523687928
C	-1.17265534391138	-0.04819702159967	-4.24695272770213
N	-0.43870064098901	-0.76347878652668	-3.35565008108404
C	0.53081509848755	-3.28996525359953	-2.14540347428744
C	-3.28229306792664	0.17681357641874	-2.90439595032720
C	-1.00062145612216	2.85141921684104	1.04585835316239
C	3.20860720305629	-0.38914596578168	1.33315476667989
C	5.17776327972397	0.68063777061575	0.31519498142082
C	-0.31608218129430	5.06700052848877	0.22975459572902
C	-3.04433987650247	1.34443133399443	-5.06164875513528
C	1.88544433287059	-3.58931677262868	-4.18991944092070
C	2.64147726957895	0.24567905071762	2.43501226392391
C	2.25091969419659	-0.48967034375934	3.54289368439827
C	2.43522280714834	-1.85949611900247	3.59962024531150
C	3.03214807475200	-2.48997061365117	2.51745374112536
C	3.40585867108369	-1.76895551753564	1.39373226618795
C	-2.36812941617639	2.61066688565535	0.94644617855831
C	-3.06046532647612	2.01746189760232	1.99111293234470
C	-2.41072228467531	1.64973081247546	3.15791508733125
C	-1.05828440156539	1.91994812189181	3.26572500054927
C	-0.35687390137646	2.51501614815727	2.23391172647268

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C    -3.47283930034707     -1.20100970248243     -2.98711857880185
C    -4.42086592856604     -1.83756927327080     -2.19400689887784
C    -5.20802189057300     -1.09443588113862     -1.32181418869245
C    -5.04741077473088      0.28034590705408     -1.26631425321585
C    -4.08867840646150      0.91532349992032     -2.04220028377643
C     1.16185722132368     -3.81451089987474     -1.02380849705242
C     0.42190014052291     -4.48753634467273     -0.06338280240132
C    -0.94427750023431     -4.64881770794642     -0.19684726519567
C    -1.58011625096261     -4.15126687857155     -1.32885748669038
C    -0.83692113322634     -3.50060583952508     -2.30399340821699
O     1.69220385996531      0.17042870312820      4.61993959223910
O    -0.39263337160492      1.65791199694545      4.44888791804430
O    -2.92765692812636     -4.33903061598570     -1.37033984434651
O    -4.69568338325461     -3.17009242200783     -2.24877413257015
C    -3.70282152499865     -4.10983612467914     -2.50793837389031
P     0.10387032266407      0.20017912545479      4.91997559427505
C     0.07636878027798      0.37526735582944      6.69753773419085
O    -0.64995160335358     -0.93247094835575      4.33879518595778
C    -0.93902701172045      1.10691426591421      7.30878467631915
C    -1.02838326230264      1.14828701330482      8.69044832868045
C    -0.10906935336919      0.45976562841700      9.46798549254065
C     0.90463862249843     -0.26859765363707      8.86301238507707
C     0.99873747422460     -0.31318519036803      7.48168807947018
H    -2.10541857900425      3.82872838183604     -4.42081733263979
H    -1.05016888995696      5.25668627706717     -2.40411350705981
H    -1.00897048843444      1.20948510251755     -1.34533687179772
H     2.42147576738650      4.98235985444163      0.00795794638979
H     4.50744764063785      3.28621498546733      0.11036209927270
H     0.96508687168392      1.06493754633118     -0.10609850747862
H     5.48431723915672     -0.53753040062943     -2.09718908485460
H     4.24326809033570     -2.13956521245508     -3.85821770313410
H     1.45009763288628     -0.87902372162062     -1.01586564200272
H     0.77445924940024     -1.92876604964778     -6.12724579688731
H    -1.15728057698837     -0.07913357827085     -6.44191452548050
H    -0.51517708724717     -0.69615177281850     -2.34830582807575
H     5.58606901430379      1.25769453552948     -0.51490816379048
H     5.34031765646828      1.23891570771968      1.23633812299028
H     5.73153477829369     -0.25427133422519      0.38328856777244
H    -1.35632149052186      5.38934429903341      0.22838774426121
H     0.10701161728840      5.28428817398459      1.20968737221494
H     0.22525341912439      5.65127687071228     -0.51425709055816
H    -3.48186944172234      0.48519687998852     -5.56745143629520
H    -3.85135571283211      2.02279993715986     -4.78937710382361
H    -2.38769940035747      1.85758703658646     -5.76381938015236
H     2.46738550403561     -3.12579428301516     -4.98608160694470
H     1.07311176259181     -4.15416522937486     -4.64511791806611
H     2.53246820767433     -4.28603248276916     -3.65914876076054
H     2.50337246259451      1.31845786064061      2.43640034542245
H     2.11960541657338     -2.42244595956794      4.46755393803410
H     3.19517795749644     -3.55929829419163      2.54669739225189
H     3.85944008506308     -2.28005723225273      0.55383512781696
H    -2.89685166414320      2.89290359426126      0.04574377328906
H    -4.12164962262741      1.82965125823483      1.89031046656711
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H	-2.94380827915401	1.17684490012187	3.97157919847834
H	0.69362959964786	2.73985480184048	2.36581575574701
H	-2.88018132941580	-1.75660948947575	-3.70200179399765
H	-5.95018691503869	-1.59689280500904	-0.71531671871512
H	-5.67566074911539	0.86556341419993	-0.60657678039643
H	-3.97587329550490	1.99077894643207	-1.99436950182857
H	2.22801208941076	-3.68670719402324	-0.89102143823335
H	0.91663386225334	-4.87562247008267	0.81766334102970
H	-1.52387078390073	-5.15142338315471	0.56610111736754
H	-1.30805616708911	-3.12353579096993	-3.19800498784309
H	-3.09916229953495	-3.85224083296989	-3.38153033758543
H	-4.24573681774288	-5.02936297658963	-2.72764989146948
H	-1.65790387811870	1.65355923309975	6.71373635837987
H	-1.81737959426773	1.71997496841915	9.16046692861734
H	-0.18083442117877	0.49423093247864	10.54731444985247
H	1.62636493122417	-0.80151128223839	9.46741527957511
H	1.80014063735195	-0.87592102063903	7.02237852079869
C	-0.93822403093932	-0.97796149105042	0.55213376357896
O	-0.37185670231824	-0.44531516498407	-0.42914589584686
N	-0.24458397851649	-1.59688872993299	1.51604855110025
H	0.75555062674279	-1.62932013394503	1.41848307427476
H	-0.58983183554014	-1.65194365530815	2.46501055570565
N	-2.27208675275618	-0.96158057110219	0.67050943692694
H	-2.83077724021018	-0.47573114815111	-0.00970738058596
H	-2.74560737493464	-1.46609093384499	1.39639024756077
H	3.93494581473119	3.02048974646448	-4.06847769120760
N	3.09717267466142	2.96933535102036	-3.51497636190908
H	3.24218704611272	3.10256520832770	-2.52526035446473
C	2.20322161981214	1.96772543582737	-3.81191732944889
N	2.16692471091822	1.62223084395015	-5.14089588525041
H	2.35300578585654	2.34404580632311	-5.81547536497167
H	1.40567842945297	1.00512904673170	-5.38217726636207
O	1.50673434076503	1.43783652562924	-2.97389405805328
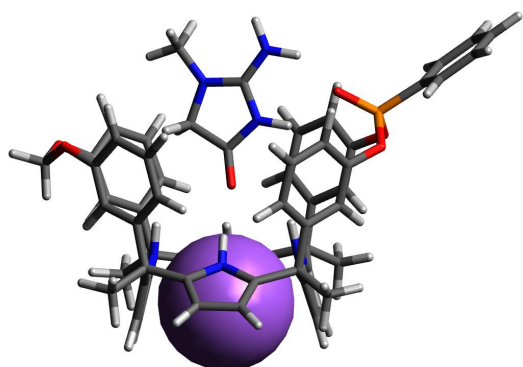
Complex **16,** $E_{tot}(Hartree)$**: -3612.032492418887**

C	2.06552369732885	4.11463073669339	-1.43682110720520
C	0.88241878535912	4.70681287138260	-1.76164243682461
C	0.96442110127655	6.07780073426508	-1.38908756972762
C	2.19657242555322	6.28889900670083	-0.84847795299468
N	2.89430249729382	5.09603363045123	-0.92036339697375
C	2.54270521035018	2.70240047852846	-1.63371493429456
C	2.83146020179288	7.54256400544289	-0.31302127886190
C	4.06372132529571	7.83217909258302	-1.14076418768662
C	4.18375107595959	8.47472480056303	-2.34896696476646
C	5.56054681939381	8.48923567202938	-2.69545827941220
C	6.25224207981698	7.85644913691477	-1.69088246593897
N	5.32151484023406	7.41975127438077	-0.78347398559132
C	7.73738105536578	7.61085632002023	-1.53964610251697
C	8.07605169341200	6.33278135662644	-2.25561527050434
C	8.95292943281498	6.07640190147207	-3.26515622982051
C	8.89936965691128	4.67996382727778	-3.54194101320695
C	7.99179503679371	4.12101249217660	-2.69519327080993
N	7.44232879470787	5.14265869159028	-1.93735823762997
C	7.48629215708876	2.70895330172338	-2.59130666855985
C	6.00818493614048	2.74368796048712	-2.91009876610514
C	5.34938744509266	2.74887026932004	-4.11497875825015
C	3.95338511339454	2.75316687777402	-3.84463787993495
C	3.79264880667006	2.75158547727957	-2.48051819595147
N	5.04805905322530	2.81159747282678	-1.93420294989279
C	7.73339491500891	2.09825195170109	-1.20679969558182
C	2.78594033553665	1.98635784807065	-0.29940301625853
C	3.16216042918158	7.42226435827709	1.17634203661705
C	8.15664982974610	7.54161276265005	-0.06888925879787
C	8.50971957620644	8.77502291348090	-2.17870261264020
C	1.83945253338860	8.70854884127325	-0.45429532564162
C	1.46384571538875	1.89996357341502	-2.37971266710906
C	8.21503303503018	1.82897889698969	-3.61817308143394
C	7.63692965443999	8.44700296867782	0.85530580659022
C	8.07135451957079	8.42393773005792	2.16916256382033
C	9.03884734032517	7.52781150381136	2.59606180054564
C	9.57444723566259	6.64897223033353	1.67055610971653
C	9.13594333180131	6.64889199593564	0.35446287444727
C	2.54069378807079	6.47617722521720	1.98463580372939
C	2.76090341513837	6.46255159527820	3.35549035374680
C	3.61279883969616	7.37957528781170	3.94737206028410
C	4.23376273627639	8.32001703902696	3.13951863192663
C	4.01340349713843	8.35147738406605	1.77398658333496

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C    3.56158276960831      0.82501483488618     -0.26398094922095
C    3.69498170657972      0.09123424328887      0.90950440234480
C    3.01788731394431      0.50031817410077      2.05720292377644
C    2.22990770793569      1.63679100497159      2.01614208385039
C    2.12868714207545      2.39485474103232      0.85541354666047
C    8.67498575052816      2.62409088871032     -0.33348016826473
C    8.92443682928053      1.99021666860551      0.87851100576016
C    8.22608564478524      0.85617035188260      1.24726326629319
C    7.27390837690379      0.31901996642236      0.37806178347441
C    7.04985486589898      0.93262174781049     -0.84813540965455
O    7.55112707038919      9.35514197595939      3.04659638966715
O    5.04928892255963      9.28428147073349      3.69453914871835
O    6.66376464344333     -0.80448685484317      0.81622099584265
O    4.39018966757795     -1.06542202703064      1.01912823863615
C    5.51058115526922     -1.34811382427367      0.23862112284244
P    6.53482952950310      8.95810459269647      4.22877827292265
C    6.81691610594699     10.19056288523307      5.46115227330158
O    6.66591808355161      7.50736793378074      4.58215771556496
C    5.77720422208467     10.56426686098530      6.31397778823633
C    6.01506486374932     11.48244607078068      7.32136912528883
C    7.28167613485535     12.02686966961888      7.48167025942881
C    8.31602463867820     11.65576313322865      6.63471862784567
C    8.09051523255558     10.73672508181310      5.62450832328414
H    0.03771799943169      4.23290037034200     -2.23350164220623
H    0.19235807946781      6.81631227275171     -1.52887840985745
H    3.65511812418258      4.88699595214541     -0.28851490702864
H    3.38252256273960      8.92734251118704     -2.91105739272232
H    5.99091589114453      8.95335200234427     -3.56830202380715
H    5.54835674693941      6.98978467830200      0.10026186903796
H    9.57199011882117      6.79518819389747     -3.77665615743796
H    9.46172916684121      4.16575756065247     -4.30391256829742
H    7.06627267369694      4.97134049874576     -1.01381611587853
H    5.80516180564726      2.70896522200359     -5.09156394224345
H    3.16560054704291      2.71913652665805     -4.57986666152013
H    5.23625641737694      2.67799026705877     -0.95307643789619
H    8.29346418980186      8.86274246447551     -3.24278993279512
H    8.24028519977392      9.71519934849191     -1.70115606857569
H    9.58248309000557      8.63153094506171     -2.05918682179253
H    0.93968503963818      8.51150525191313      0.12688649578800
H    2.28039127301168      9.63337494684354     -0.08829636451127
H    1.54796165907825      8.86306754878760     -1.49220829052062
H    1.81506837817711      0.88996069212211     -2.58117943343444
H    0.55861303493745      1.82795032956686     -1.77935870327257
H    1.20809368830800      2.36586256486115     -3.33029157957993
H    8.06459238335322      2.18765577709059     -4.63573569238426
H    7.85534623678412      0.80345894379432     -3.56670995456680
H    9.28515372458075      1.81799387771855     -3.41557014414245
H    6.92320015094604      9.20293939039574      0.55016472285440
H    9.39341087621390      7.54065691764027      3.61764446675181
H   10.35673896200611      5.96666860136788      1.97492941108479
H    9.59818663828241      5.97543029526480     -0.35550784378077
H    1.84100973001853      5.77227838720395      1.55324517273422
H    2.23932481161331      5.74439053461886      3.97447946560282
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H    3.76178953608147      7.38812168515407       5.01886636339448
H    4.47340262966448      9.13674292137436       1.18617017002385
H    4.00610700475238      0.47039023116588      -1.18526978770225
H    3.07378936859810     -0.10927920374686       2.95009912969223
H    1.66992494699958      1.92716844728105       2.89592723970413
H    1.47931706486656      3.26079755222625       0.83210302605407
H    9.24638085005916      3.50079897517010      -0.60603947817828
H    9.68656299327487      2.38208391941953       1.53947158389024
H    8.43713731525859      0.35084140122365       2.18132976972187
H    6.36408484676945      0.49562552415345      -1.56252810506708
H    5.38218089705230     -1.05068283243356      -0.80483548916116
H    5.62598504687177     -2.42849588164795       0.27851561539119
H    4.78018763992195     10.16315426682750       6.18870047916775
H    5.20891028667586     11.78133983775726       7.97692915342696
H    7.46031727704371     12.74924900092583       8.26660084778533
H    9.29890963744523     12.08988743588658       6.75466329846608
H    8.90203130945670     10.46978439026481       4.96123056969661
N    5.82776146166364      3.15142854607632       3.96441662529929
C    6.13501214137211      4.40417623628246       4.24505120601578
N    6.13076438882859      5.15679489469090       3.11221227074814
C    5.79696042139650      4.40220977916764       2.02320678002588
C    5.60489980025395      3.00082820244568       2.53921250075188
O    5.68176135935475      4.79195153180344       0.88704571329479
N    6.41061072562168      4.92192261687912       5.41369533350170
C    5.77644601023693      2.05802946919087       4.91263537215032
H    6.58704357058013      5.93097361965407       5.45797066528481
H    6.44168006817842      4.36740553190967       6.25296763924419
H    5.26829598449209      1.21874237483115       4.44644377765478
H    5.20392265026865      2.33627435027951       5.79706316103394
H    6.77432177874391      1.73404339710729       5.20814538905064
H    6.33100424828618      2.32095285860364       2.08230536275960
H    4.59739063479213      2.63481616535261       2.32114371373131
H    6.31664021178557      6.16038714796858       3.15133586887523
Na   4.88538387977030      5.47151750871518      -2.83818675693475
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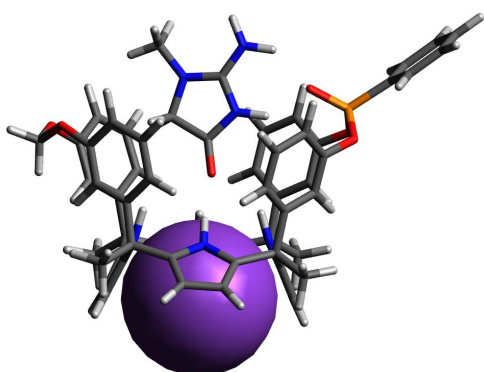
Complex **17**, $E_{tot}(Hartree)$: **-4049.466286488017**

C	2.10745558653347	4.13084517102189	-1.47722227594092
C	0.96252248733760	4.73665373748820	-1.91182667956949
C	1.04036495897166	6.11165955198505	-1.56830404127786
C	2.23244154889967	6.31604283268961	-0.93370177212744
N	2.90030138039849	5.11017155975376	-0.91689759675063
C	2.55196345879193	2.69660893378161	-1.59549639996640
C	2.82632073774646	7.57720414177095	-0.36314478013225
C	4.06580892330326	7.92978274537489	-1.15315224073381
C	4.21342438628496	8.72127889375560	-2.26437343402139
C	5.59117148667833	8.73525844786043	-2.60374275249460
C	6.25388728792110	7.95106561792713	-1.69263233658316
N	5.30640350191852	7.43388910285603	-0.84795440439102
C	7.72607192619200	7.63483671205865	-1.56386181113366
C	8.01122831419359	6.34775866069993	-2.29369958634833
C	8.79058189860831	6.10319374675384	-3.38929993326488
C	8.73950392161277	4.70925599523241	-3.65493710310872
C	7.92849793938844	4.13423978000133	-2.71747381415789
N	7.45168675746877	5.14707960819094	-1.91351237704030
C	7.48242138329177	2.70290062537185	-2.56607905636863
C	6.00716075836429	2.63785249413200	-2.88374158605133
C	5.35115962104162	2.37477387605272	-4.05841191299547
C	3.95675362434683	2.37843664418488	-3.78470224425864
C	3.79490599811976	2.64434983521863	-2.44915434429242
N	5.04618566304810	2.85983619268719	-1.93121375974945
C	7.75679279756118	2.14168923827080	-1.16557752846576
C	2.78562486823696	2.04767236948188	-0.22602686872147
C	3.13770397931466	7.43821588623442	1.12900758516342
C	8.15561914918337	7.54713822164881	-0.09728510635989
C	8.54110733520532	8.76814036600503	-2.20452272648911
C	1.80182264153185	8.71527799530366	-0.49621233565280
C	1.44207290287613	1.88434110723869	-2.28154009216118
C	8.25571644356430	1.82629619576199	-3.56245032679868
C	7.62309666294518	8.42312002674723	0.84685368913222
C	8.07550599167749	8.39312670432130	2.15429307580638
C	9.06664451465955	7.51337526699698	2.55779501206067
C	9.61214148192158	6.66077768982535	1.61287444793972
C	9.16112763300749	6.67198894610116	0.30116344374451
C	2.49021945367667	6.49732166505378	1.92289663582875
C	2.70400389940301	6.46156018785122	3.29418622774859
C	3.57217436087343	7.35355196347926	3.90083885310811
C	4.21258222687450	8.29294667525193	3.10758603457448
C	4.00151585293740	8.34491551446304	1.74171408099786

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C    3.58707449131211      0.90850198444257     -0.12603432924510
C    3.70303989919734      0.22049933278426      1.07640949803008
C    2.98327963849991      0.65502032263846      2.18853108094196
C    2.17694635157296      1.77524775577115      2.08562534166080
C    2.09060661222478      2.48698446273202      0.89505293497951
C    8.74410660806102      2.67390963239842     -0.34777044476279
C    9.03103607095567      2.07102981683832      0.87150312573050
C    8.32688696918949      0.96215617355789      1.30188471228410
C    7.32626064793901      0.42221586546217      0.49126400947762
C    7.06238093504151      1.00453913993665     -0.74187233852054
O    7.54951295025984      9.30408323120793      3.05158239808436
O    5.04205572627137      9.23644200712140      3.67975944129950
O    6.70364814851580     -0.66702418914772      0.99738544109131
O    4.43326362913288     -0.90583877082478      1.25484948709581
C    5.53730133567440     -1.27775416897269      0.46507990953171
P    6.52026368725395      8.88211997072291      4.21192277692211
C    6.80423978538682     10.06835682882084      5.48874471479057
O    6.63894071556430      7.41988453594285      4.52693765714968
C    5.75426810027061     10.44925360515141      6.32550381234437
C    5.99461393716474     11.32489549687829      7.36973583003198
C    7.27358249995520     11.82001128863409      7.58213567936291
C    8.31801865451803     11.44273923309170      6.75027520645234
C    8.09001368497464     10.56628825556349      5.70347788891347
H    0.14314510647699      4.25966638783175     -2.42346284590734
H    0.28913064376984      6.85700355035536     -1.77060024995264
H    3.67336804992582      4.92190191910093     -0.29670934073284
H    3.43159317382154      9.26937935590771     -2.76473274796919
H    6.03970509141239      9.30056121766313     -3.40473585479469
H    5.51960485683295      6.92020143486334     -0.00543503408723
H    9.35296453977098      6.83182925243961     -3.94986873793143
H    9.24655672019377      4.20012756357238     -4.45781777591474
H    7.04452775288867      4.98405098998948     -1.00472836968055
H    5.80935497920083      2.15515147874573     -5.00903186514082
H    3.17333387460503      2.16284657344595     -4.49347402295785
H    5.24160136620802      2.89291040066893     -0.94301406949322
H    8.32157466299604      8.86920857015342     -3.26688284966246
H    8.31536736657532      9.71658849049829     -1.72078397034044
H    9.60783499584944      8.57875427436089     -2.09575405974998
H    0.89644647782605      8.47298920321341      0.05800385274145
H    2.20592616289520      9.64243681578229     -0.09513049539638
H    1.52638278955436      8.89093787837205     -1.53542338659275
H    1.75532860260166      0.85057651444321     -2.41360997595393
H    0.53787614225355      1.88673387648403     -1.67524048604191
H    1.19679087058792      2.29286793970146     -3.26097531091937
H    8.08823120180312      2.14057992740063     -4.59216604650076
H    7.94714331908258      0.78670684916362     -3.47383991760940
H    9.32459231227627      1.87847691881447     -3.36176958050831
H    6.88595927814694      9.16492642800328      0.56401444004445
H    9.43086090374476      7.51866954831529      3.57634324748952
H   10.41201306872739      5.99093203751250      1.89882534008938
H    9.63037108101221      6.01974147690195     -0.42402470888325
H    1.77988247394143      5.81221178972507      1.47921556459313
H    2.16765754878199      5.74452229105568      3.90166466033692
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H    3.71912832095972        7.34413063804634        4.97273732368195
H    4.47989776412174        9.12733167722712        1.16479772892960
H    4.06416035636825        0.53178827555976       -1.02118810952993
H    3.02629569186977        0.08132721563624        3.10579505246350
H    1.59162822046130        2.08815080078538        2.94076582694176
H    1.42829666467879        3.34041663874652        0.82351002753337
H    9.32001987511981        3.52974915803644       -0.67206962208556
H    9.82604996129969        2.46685924646159        1.48998018025307
H    8.56376141344840        0.48139193266176        2.24269879386803
H    6.34080260397833        0.56373718070020       -1.41674778441018
H    5.39068209814238       -0.97426524255202       -0.58667263918985
H    5.64900623452964       -2.30594205198165        0.54969461074805
H    4.74831610613763       10.08715088848062        6.15985655311242
H    5.18095994889713       11.62953556086428        8.01330211476202
H    7.45455106930808       12.50959836561437        8.39549722263788
H    9.31081329107362       11.83959164415866        6.91080442370606
H    8.91006406106846       10.29464877849656        5.05241360693741
N    5.85054975932530        3.09341486652687        3.88867366084519
C    6.14718519361605        4.33323078651158        4.22757337913189
N    6.14937728606198        5.14015449244470        3.13395152233789
C    5.82734588233127        4.43569665743417        2.01067486859087
C    5.64424228396745        3.01101357408780        2.45620536159399
O    5.71204720362905        4.87241241362853        0.89043009304080
N    6.40860296195620        4.79544030819114        5.42454366710772
C    5.79340512871703        1.95479412117146        4.78194458008177
H    6.58299276437654        5.79605694212840        5.52306163615088
H    6.43315705897714        4.20141720381614        6.23638771984359
H    5.30875259147530        1.13291178114903        4.26278238168507
H    5.19700951609739        2.18262081728172        5.66509767514643
H    6.78889674841763        1.62953111463462        5.08383786117823
H    6.38492138565147        2.36309955556813        1.97823300496133
H    4.64382386763150        2.64541883137133        2.21148970593092
H    6.32979965198891        6.14728656623675        3.23894361511272
K    4.76522594699331        5.59459307879538       -3.31637565511459
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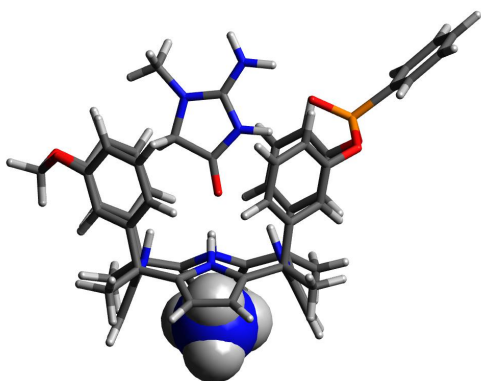
Complex **18**, $E_{tot}(Hartree)$: **-3506.976474525024**

C	1.87149088347481	4.34128948372045	-2.73037188460173
C	0.76515495943532	4.88741194352370	-3.32258525973660
C	0.82217649287675	6.29204550545202	-3.13534807549148
C	1.96340677871614	6.57236240152513	-2.43460719413141
N	2.61001896150158	5.38034507467226	-2.21736641797956
C	2.32883127599377	2.90735403575910	-2.65912930963040
C	2.51607256227075	7.88837652192008	-1.95422754816523
C	3.84444352489933	8.14031591062382	-2.63138422960960
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