Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

for

Coronene-based quantum dots for delivery of the doxorubicin anticancer drug: A computational study †

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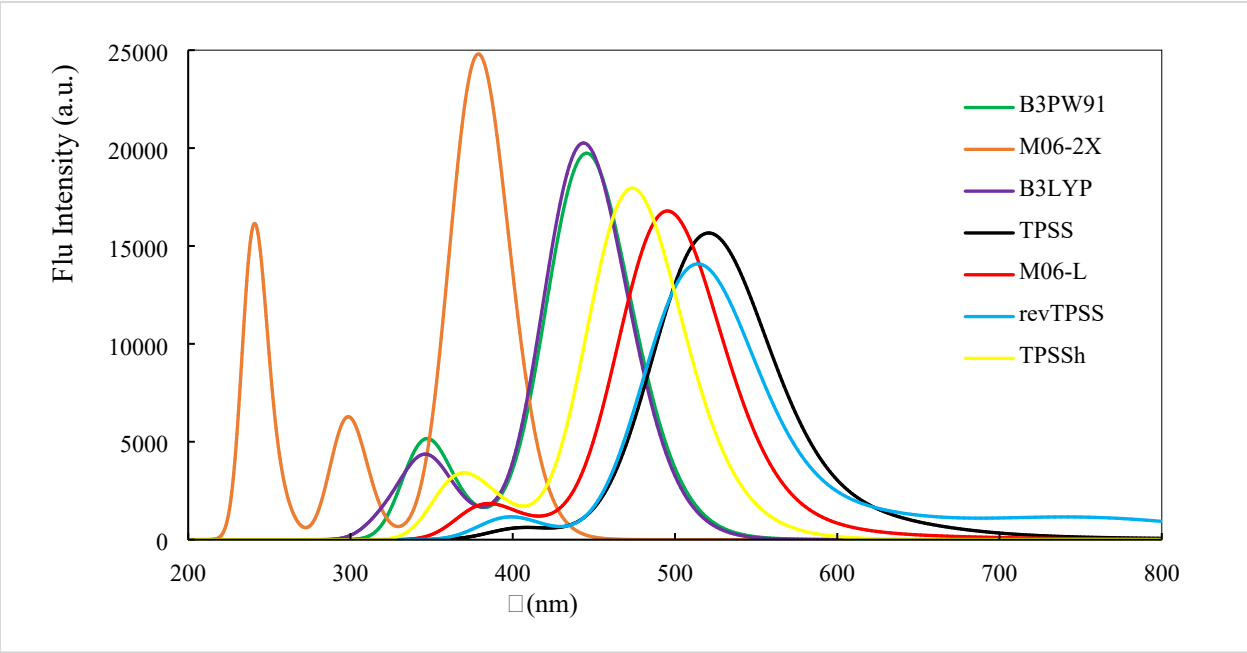

Fig. S1. Emission spectra of DOX at different levels of theory. The experimental emission wavelength is 560nm.

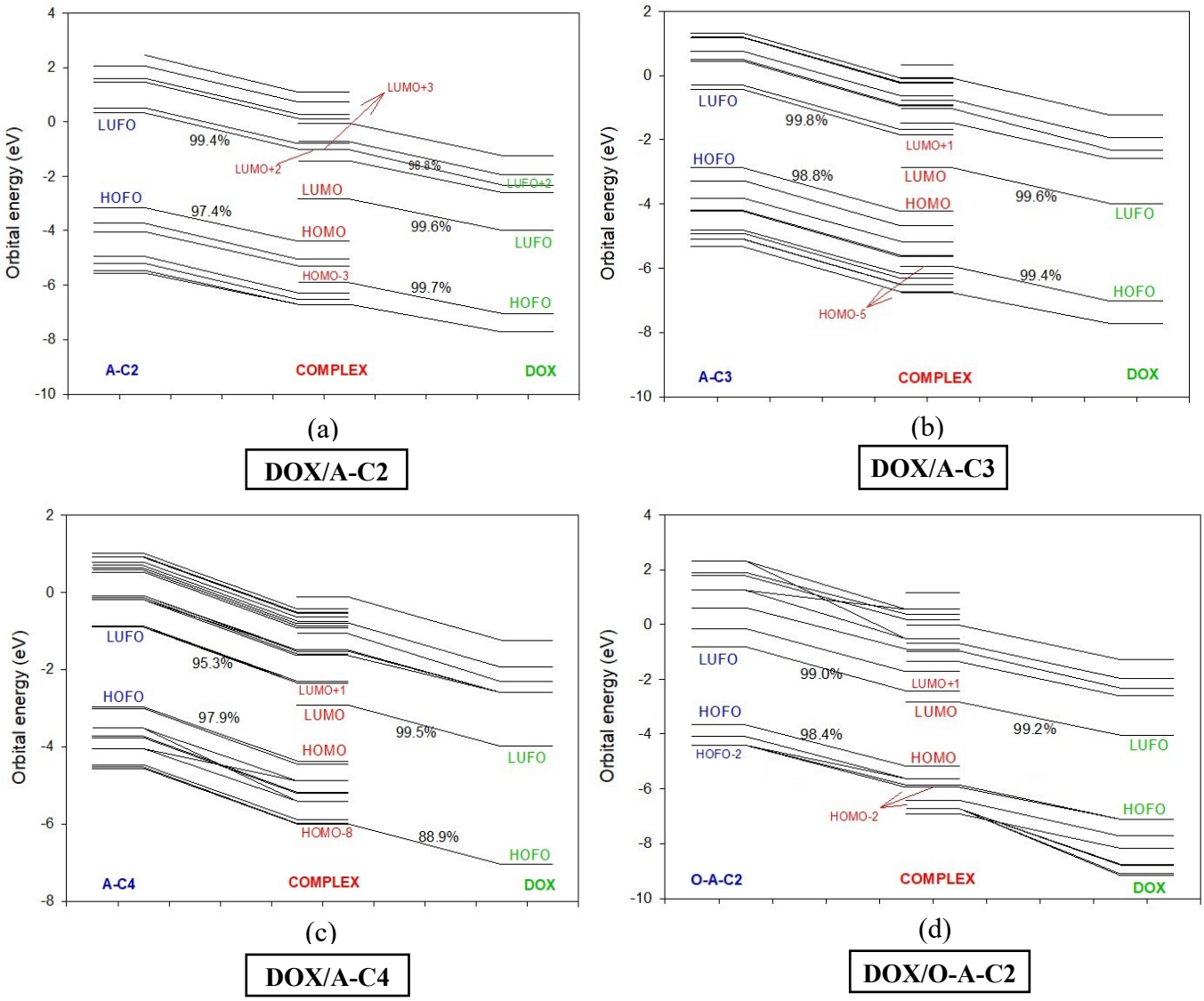

Fig. S2. Orbital interaction diagrams using CDA analysis for (a) DOX/A-C2, (b) DOX/A-C3, (c) DOX/A-C4, and (d) DOX/O-A-C2 complexes.

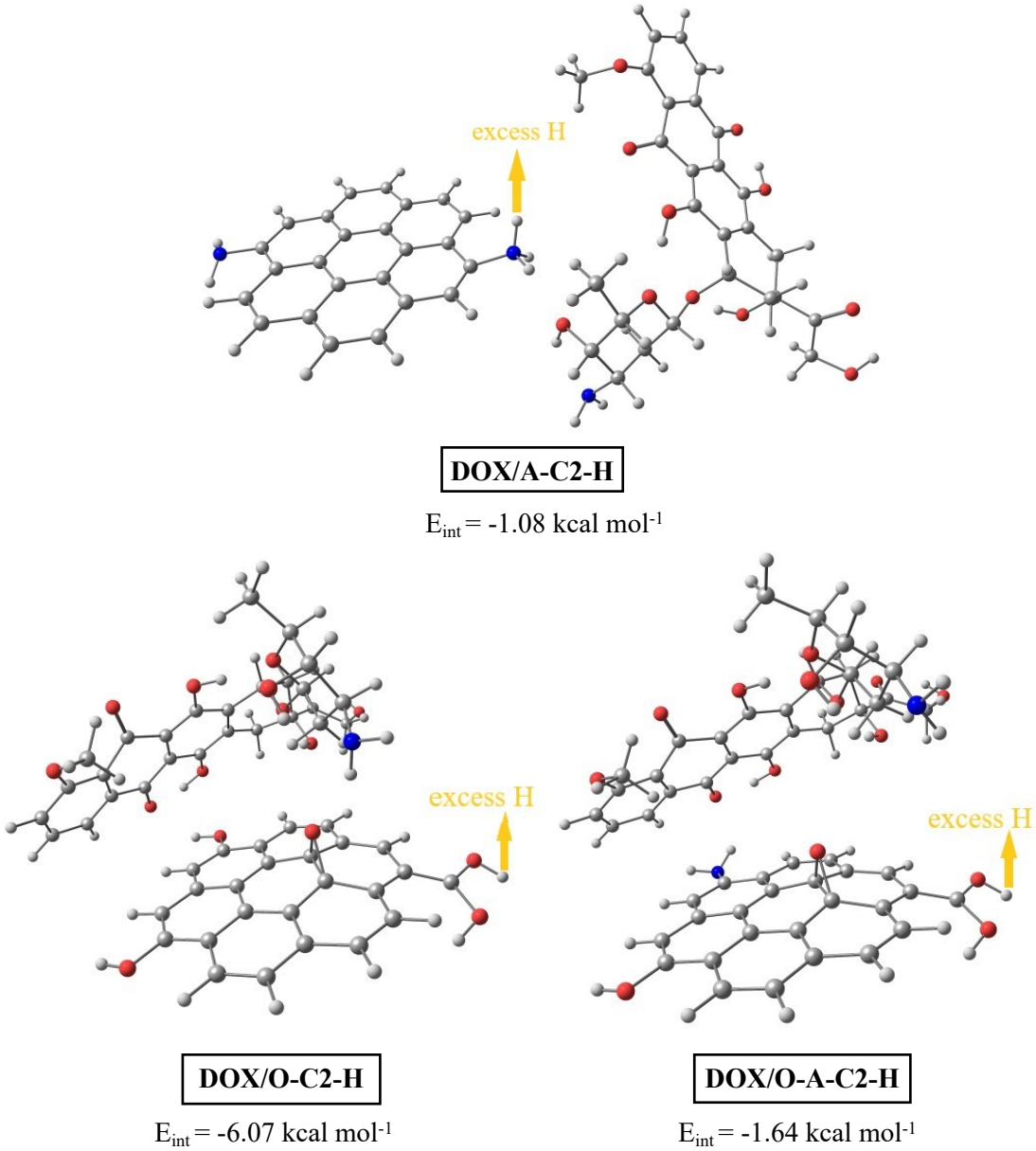

Fig. S3. The optimized structure of DOX/CCs in the presence of H^+.

Table S1. QTAIM topological parameters at BCPs of interaction contacts in considered systems (au).

Complex	BCP	R(Å)	$\rho(r)$	$\nabla^2\rho(r)$	$G(r)$	$V(r)$	$H(r)$	$G(r)/\|V(r)\|$
DOX/A-C2	O…H	2.69	0.0060	0.0227	0.0047	-0.0037	0.0010	1.2622
	O…H	2.17	0.0158	0.0529	0.0130	-0.0128	0.0002	1.0177
	O…H	2.50	0.0083	0.0339	0.0074	-0.0064	0.0011	1.1655
	N…H	3.29	0.0022	0.0076	0.0014	-0.0009	0.0005	1.5559
	O…H	2.31	0.0124	0.0433	0.0104	-0.0100	0.0004	1.0400
	O…H	2.35	0.0112	0.0416	0.0094	-0.0085	0.0010	1.1142
DOX/O-C2	O…H	2.38	0.0107	0.0366	0.0085	-0.0079	0.0006	1.0807
	O…H	2.40	0.0100	0.0417	0.0093	-0.0081	0.0012	1.1440
	O…H	2.47	0.0097	0.0317	0.0073	-0.0066	0.0006	1.0975
	O…H	2.91	0.0098	0.0379	0.0088	-0.0081	0.0007	1.0855
	O...H	1.80	0.0355	0.1098	0.0285	-0.0295	-0.0010	0.9647
DOX/O-A-C2	O…H	2.12	0.0179	0.0570	0.0143	-0.0144	-0.0001	0.9948
	O…H	3.09	0.0024	0.0098	0.0018	-0.0011	0.0007	1.6507
	O…H	2.63	0.0075	0.0281	0.0059	-0.0048	0.0011	1.2313
	O…H	2.34	0.0121	0.0398	0.0096	-0.0093	0.0003	1.0342
	O…N	3.32	0.0052	0.0205	0.0043	-0.0035	0.0008	1.2262
DOX/A-C3	O…H	2.79	0.0056	0.0215	0.0043	-0.0033	0.0010	1.3121
	O…H	2.13	0.0174	0.0563	0.0141	-0.0141	0.0000	0.9977
	O…H	2.54	0.0078	0.0333	0.0071	-0.0060	0.0012	1.1960
	O…H	2.32	0.0122	0.0423	0.0102	-0.0098	0.0004	1.0415
	O…H	2.42	0.0100	0.0383	0.0085	-0.0074	0.0011	1.1480
	N…H	3.02	0.0041	0.0127	0.0025	-0.0019	0.0006	1.3319
DOX/A-C4	O…H	2.69	0.0057	0.0227	0.0047	-0.0036	0.0010	1.2818
	O…H	2.19	0.0167	0.0524	0.0134	-0.0138	-0.0003	0.9767
	N…H	3.02	0.0039	0.0125	0.0025	-0.0019	0.0006	1.3478
	O…H	2.57	0.0074	0.0317	0.0068	-0.0056	0.0012	1.2057
	O…H	2.20	0.0151	0.0489	0.0121	-0.0120	0.0001	1.0093
	O…H	2.70	0.0064	0.0245	0.0050	-0.0040	0.0011	1.2713
	O…H	3.30	0.0015	0.0061	0.0011	-0.0006	0.0005	1.7716

Table S2. Wavelength (λ), and major orbital contributions to the crucial electronic transitions for all studied systems.

Systems	Transitions	λ (nm)	Major contributions Hole → Electron (%)
DOX	$S_0 \rightarrow S_3$	521	H-1>L (10%), H>L (74%)
A-C2	$S_0 \rightarrow S_8$	325	H-5>L (10%), H-1>L+1 (59%), H>L (11%)
A-C3	$S_0 \rightarrow S_8$	474	H-1>L (56%), H>L+1 (20%)
A-C4	$S_0 \rightarrow S_6$	656	H-1>L (19%), H-1>L+1 (22%), H>L (15%), H>L+1 (14%)
O-C2	$S_0 \rightarrow S_5$	380	H-1>L+1 (22%), H>L+1 (19%), H>L+2 (26%)
O-A-C2	$S_0 \rightarrow S_6$	388	H-1>L+1 (26%), H>L+1 (13%), H>L+2 (28%)
DOX/A-C2	$S_0 \rightarrow S_8$	522	H-3>L (74%)
DOX/A-C3	$S_0 \rightarrow S_4$	702	H-1>L+2 (20%), H>L+1 (77%)
DOX/A-C4	$S_0 \rightarrow S_5$	820	H-1>L+1 (29%), H>L+2 (56%)
DOX/O-C2	$S_0 \rightarrow S_6$	548	H-6>L (14%), H-5>L (42%), H-2>L (37%)
DOX/O-A-C2	$S_0 \rightarrow S_9$	604	H-6>L (52%), H-3>L (18%)

Table S3. The recovery time of DOX/CC complexes (Seconds) in the absence of radiation at room temperature (298 K), body temperature (310 K), and cancer tissue temperature (315 K) in the gas and the solvent phase.

system	Gas			Water		
	Room temperature	Body temperature	Cancer cell temperature	Room temperature	Body temperature	Cancer cell temperature
DOX/A-C2	5.66E+03	4.05E+03	3.55E+03	1.59E+04	1.10E+04	9.45E+03
DOX/A-C3	3.09E+04	2.07E+04	1.77E+04	1.72E+05	1.08E+05	8.95E+04
DOX/A-C4	1.36E+05	8.59E+04	7.18E+04	2.49E+05	1.54E+05	1.27E+05
DOX/O-C2	7.15E+05	4.24E+05	3.45E+05	1.99E+06	1.13E+06	9.08E+05
DOX/O-A-C2	3.99E+03	2.90E+03	2.55E+03	4.84E+03	3.49E+03	3.06E+03

Cartesian coordinates (Å) for the studied compounds in gas phase

DOX

	X	Y	Z
C	7.154572	0.764032	0.139183
C	6.070704	1.584357	0.432917
C	4.770721	1.074477	0.3459
C	4.530974	-0.273209	0.000188
C	5.643003	-1.088842	-0.309625
C	6.937064	-0.558522	-0.24241
H	8.166981	1.154714	0.191216
H	6.202338	2.622725	0.715227
H	7.764522	-1.207708	-0.513282
C	2.276961	1.54596	0.301141
C	1.2224	2.47888	0.37443
C	-0.092545	2.098913	0.014333
C	-0.326483	0.794775	-0.405351
C	0.71328	-0.181418	-0.411585
C	2.021152	0.194297	-0.070709
C	3.129056	-0.807631	-0.003974
C	3.640312	2.000473	0.592948
C	-1.165974	3.162708	0.061358
C	-2.602093	2.621937	-0.086862
C	-2.622946	1.554013	-1.200065
C	-1.704654	0.379448	-0.864074
H	-0.978462	3.897956	-0.731708
H	-3.643704	1.183012	-1.352841
O	5.509438	-2.367444	-0.775647
O	3.868548	3.160673	0.99178
O	2.916529	-2.008678	0.08852
O	0.477295	-1.439995	-0.838013
O	1.400896	3.75394	0.757589
H	-0.436919	-1.742152	-0.658159
H	2.371306	3.848268	0.966688
C	5.566074	-3.404779	0.209028
H	5.516518	-4.344438	-0.344832
H	6.510286	-3.360911	0.769022
H	4.713767	-3.334965	0.889211
O	-3.293604	4.456398	-1.478332

	C	-3.533498	3.766794	-0.499476
	C	-4.789426	4.031168	0.312598
	H	-5.374053	3.100053	0.366851
	H	-4.487099	4.250832	1.348889
	O	-5.539741	5.075139	-0.245685
	H	-5.013596	5.39368	-1.004902
	O	-3.102958	2.10452	1.142565
	H	-2.829909	1.172347	1.210855
	O	-2.290605	-0.407918	0.225979
	C	-3.057231	-1.5094	-0.17113
	C	-3.829012	-2.038472	1.027896
	C	-4.563136	-3.331513	0.649226
	H	-3.112181	-2.242286	1.829395
	C	-2.747258	-3.717818	-1.088733
	C	-3.56533	-4.34986	0.047174
	O	-2.143179	-2.483993	-0.65469
	O	-2.69891	-4.822915	1.053362
	N	-5.140548	-3.943525	1.854857
	C	-1.623192	-4.608406	-1.593518
	H	-1.062817	-4.100033	-2.383805
	H	-0.94429	-4.852169	-0.773438
	H	-2.033079	-5.539774	-1.998122
	H	-5.854877	-4.624942	1.602203
	H	-5.593882	-3.242417	2.437498
	H	-3.256762	-4.855855	1.857172
	H	-4.535364	-1.274164	1.374979
	H	-3.743427	-1.233442	-0.993456
	H	-5.321914	-3.096936	-0.117584
	H	-4.143282	-5.182813	-0.397589
	H	-3.445715	-3.48514	-1.911164
E= - (Hartree)	H	-1.092757	3.709005	1.007467
	H	-1.609979	-0.276921	-1.735791
	H	-2.298458	2.017147	-2.138255

1928.5185207

A-C2

	X	Y	Z
C	0.238497	3.738413	-0.036924
C	-0.777244	2.740509	-0.032034
C	-2.160889	3.061015	-0.06072
C	-2.768945	0.701065	-0.000245
C	-3.121191	2.079516	-0.04893
C	-3.754403	-0.346806	0.043663
C	1.983158	2.037636	-0.008226
C	1.567468	3.40075	-0.023255
C	0.989775	1.021924	-0.005902
C	-0.393683	1.371099	-0.012643
C	-0.989774	-1.021923	-0.005901
C	-1.391548	0.347918	-0.002637
C	-1.983153	-2.03764	-0.008222
C	-3.351037	-1.667685	0.029324
C	3.754401	0.346794	0.043664
C	3.35103	1.667685	0.029319
C	2.768943	-0.70106	-0.000249
C	1.391548	-0.347912	-0.002643
C	0.77724	-2.740507	-0.032035
C	0.39368	-1.371098	-0.012645
C	-0.238488	-3.738408	-0.03692
C	-1.567466	-3.400743	-0.023251
C	3.121185	-2.079524	-0.04893
C	2.160899	-3.061012	-0.060724
H	-4.101829	-2.455473	0.059303
H	-2.454091	4.107407	-0.103744
H	-0.059419	4.78427	-0.052511
H	2.328545	4.177568	-0.025318
H	4.10183	2.455465	0.059285
H	4.16676	-2.363914	-0.114271
H	2.45409	-4.107407	-0.103749
H	0.059418	-4.784267	-0.052505
H	-2.328535	-4.177569	-0.025314
N	5.114223	0.008906	0.04365
H	5.349204	-0.78848	0.623064
H	5.722078	0.790715	0.259173
H	-4.166755	2.363913	-0.114271
N	-5.114227	-0.008888	0.043635
H	-5.34919	0.788364	0.623246
H	-5.722089	-0.790736	0.259019

E= -1032.601577 (Hartree)

A-C3

	X	Y	Z
C	2.829087	-4.909814	0.03212
C	1.430422	-4.931366	0.015653
C	0.681128	-6.157233	0.007835
C	-1.430264	-4.931412	-0.01642
C	-0.6809	-6.15728	-0.008761
C	-2.829002	-4.90993	-0.032819
C	5.668257	-2.499534	0.046981
C	4.982238	-3.677654	0.061639
C	2.848287	-2.46254	0.020244
C	3.550302	-3.708702	0.034646
C	1.426111	-2.463627	0.01189
C	0.713115	-3.693265	0.006071
C	-1.425979	-2.463672	-0.012483
C	-0.712922	-3.693257	-0.006788
C	-2.848211	-2.462538	-0.02051
C	-3.550346	-3.708781	-0.034976
C	-5.668463	-2.49957	-0.04659
C	-4.982384	-3.677734	-0.061879
C	5.701152	-0.000079	-0.048899
C	4.996942	-1.23035	0.004665
C	2.851648	-0.000004	0.007415
C	3.567331	-1.226997	0.016972
C	1.423603	0.000011	0.007685
C	0.710188	-1.227484	0.001057
C	-1.423508	0.000014	-0.008528
C	-0.710035	-1.227492	-0.001865
C	-2.851552	0.00003	-0.007596
C	-3.567307	-1.226992	-0.016757
C	-5.701273	-0.000078	0.050977
C	-4.99693	-1.230431	-0.003768
C	5.668397	2.499598	0.048605
C	4.996995	1.230345	0.005361
C	2.848322	2.462615	0.020474
C	3.567331	1.227017	0.017223
C	1.426134	2.463674	0.011734
C	0.710192	1.227524	0.000895
C	-1.42612	2.463663	-0.012971

C	-0.71006	1.22753	-0.002106
C	-2.848359	2.462545	-0.020903
C	-3.567417	1.226972	-0.016966
C	-5.668533	2.499569	-0.045703
C	-4.997114	1.230352	-0.003549
C	4.982296	3.677728	0.06323
C	2.829105	4.909923	0.032613
C	3.550361	3.708775	0.03531
C	1.430394	4.931482	0.01548
C	0.713039	3.693315	0.005715
C	-1.430411	4.931499	-0.017163
C	-0.71304	3.693316	-0.007383
C	-2.829166	4.909936	-0.033468
C	-3.550449	3.708771	-0.035323
C	-4.982464	3.677705	-0.061394
C	0.681048	6.157387	0.007416
C	-0.681026	6.157397	-0.009542
H	-6.751976	2.534226	-0.109104
H	-6.751822	-2.533805	-0.111274
H	-5.52042	-4.621546	-0.104574
H	-3.373372	-5.852011	-0.043523
H	-1.229838	-7.095933	-0.015537
H	1.230011	-7.095878	0.014402
H	3.37344	-5.851858	0.042649
H	5.520242	-4.621472	0.103889
H	6.751647	-2.533921	0.111455
H	6.75169	2.533663	0.114155
H	5.520231	4.621567	0.105931
H	3.373354	5.852039	0.043405
H	1.229942	7.096042	0.014116
H	-1.229933	7.096063	-0.016415
H	-3.37351	5.852019	-0.044113
H	-5.520565	4.621494	-0.103408
N	-7.0974	-0.000764	0.109885
H	-7.498725	0.828546	0.526951
H	-7.49743	-0.827736	0.532894
N	7.097271	-0.000114	-0.106779
H	7.498395	0.827901	-0.526669
H	7.498403	-0.828523	-0.525738

E= -2179.6457101 (Hartree)

A-C4

	X	Y	Z
C	-8.439242	1.914003	-0.038551
C	-8.661643	0.563712	-0.060063
C	-5.360947	5.806516	0.035232
C	-5.596235	4.409022	0.027412
C	-6.899013	3.854697	0.022413
C	-5.994367	1.586721	0.000405
C	-7.121262	2.48034	0.007081
C	-6.205154	0.18157	-0.010176
C	-7.536552	-0.365042	-0.017849
C	-6.613652	-2.641482	0.02661
C	-7.70793	-1.742425	0.022406
C	-6.787217	-4.045599	0.047509
C	-2.565945	8.266648	0.027685
C	-3.828245	7.762679	0.035302
C	-2.941694	5.458315	0.024024
C	-4.077343	6.340881	0.03232
C	-3.149305	4.053119	0.020214
C	-4.469323	3.523706	0.019826
C	-3.556392	1.231355	0.004034
C	-4.67755	2.115493	0.010797
C	-3.76189	-0.171197	0.001863
C	-5.089323	-0.700397	-0.003335
C	-4.170103	-2.991948	0.008752
C	-5.286289	-2.109528	0.007675
C	-4.371167	-4.397522	0.021594
C	-5.709293	-4.922352	0.041421
C	-4.808162	-7.196891	0.044207
C	-5.875166	-6.355466	0.053037
C	-0.108499	7.903347	0.006764
C	-1.406623	7.407213	0.017697
C	-0.504782	5.1083	0.010325
C	-1.622039	5.985059	0.017873
C	-0.710628	3.695227	0.010527
C	-2.027235	3.169792	0.012041
C	-1.118128	0.881329	0.002168
C	-2.233334	1.760294	0.008638
C	-1.323617	-0.5277	0.001546

C	-2.642962	-1.053597	-0.00115
C	-1.731414	-3.340936	-0.000935
C	-2.844548	-2.463281	0.002209
C	-1.935827	-4.754151	0.004196
C	-3.255477	-5.277425	0.016682
C	-2.349546	-7.546473	0.016617
C	-3.453102	-6.701713	0.025435
C	2.349465	7.546481	-0.017628
C	1.022889	7.051754	-0.002639
C	1.935779	4.754211	-0.004384
C	0.817254	5.63369	0.001652
C	1.7314	3.341003	0.00117
C	0.408388	2.814266	0.004309
C	1.323609	0.52776	-0.000924
C	0.204867	1.409019	0.004954
C	1.118132	-0.881275	-0.001259
C	-0.204865	-1.408952	-0.004265
C	0.710639	-3.695149	-0.010153
C	-0.408387	-2.814205	-0.00378
C	0.504798	-5.108242	-0.010153
C	-0.817265	-5.63362	-0.001848
C	0.108519	-7.903334	-0.007379
C	-1.022901	-7.05173	0.002046
C	4.808031	7.196963	-0.045762
C	3.453011	6.701761	-0.026487
C	4.371093	4.397603	-0.022233
C	3.255401	5.277509	-0.017279
C	4.170085	2.992023	-0.008837
C	2.844528	2.463342	-0.002062
C	3.761854	0.17122	-0.001469
C	2.642946	1.053658	0.001819
C	3.556376	-1.231335	-0.003202
C	2.233321	-1.760238	-0.008051
C	3.149309	-4.053022	-0.019824
C	2.027239	-3.169726	-0.011293
C	2.941747	-5.458208	-0.023826
C	1.622081	-5.98497	-0.01787
C	2.566034	-8.266556	-0.028153
C	1.406691	-7.40714	-0.018039
C	5.875064	6.355572	-0.054665
C	6.787182	4.045666	-0.048745

C	5.709223	4.922447	-0.042599
C	6.613635	2.641498	-0.027287
C	5.286262	2.109546	-0.007825
C	6.20515	-0.181636	0.010517
C	5.089303	0.70038	0.003707
C	5.994336	-1.586784	0.000198
C	4.67751	-2.115463	-0.01027
C	5.596149	-4.408969	-0.027198
C	4.469316	-3.523664	-0.019307
C	5.360911	-5.806364	-0.035295
C	4.077355	-6.340747	-0.032376
C	3.828313	-7.762525	-0.035653
C	7.707937	1.742346	-0.022915
C	8.661822	-0.564087	0.060622
C	7.536585	0.364903	0.017991
C	8.439229	-1.914297	0.038985
C	7.121168	-2.48045	-0.00649
C	6.898917	-3.854692	-0.022128
H	6.886656	6.753525	-0.070599
H	7.798087	4.447033	-0.066711
H	8.706352	2.164246	-0.083608
H	9.286568	-2.596676	0.076899
H	7.752204	-4.529998	-0.025388
H	6.215984	-6.479478	-0.041383
H	4.685328	-8.431967	-0.043101
H	-6.886753	-6.753419	0.068572
H	-7.798098	-4.447001	0.06505
H	-8.706425	-2.164279	0.082155
H	-9.286707	2.596261	-0.076074
H	-7.752368	4.529966	0.025363
H	-6.216065	6.479625	0.041142
H	-4.685271	8.432137	0.042611
H	-2.405703	9.342103	0.028946
H	0.048294	8.979901	0.005113
H	2.504866	8.62325	-0.023049
H	4.959052	8.273701	-0.054027
H	2.405798	-9.342023	-0.029659
H	-0.048263	-8.979913	-0.006016
H	-2.504939	-8.623267	0.021732
H	-4.959201	-8.273641	0.052157
N	9.955965	-0.033303	0.069681

N	-9.955592	0.032451	-0.06763
H	-10.6737	0.723227	-0.253367
H	-10.07473	-0.772369	-0.671925
H	10.076082	0.770559	0.67501
H	10.674732	-0.724249	0.252416

E= -3784.107974 (Hartree)

O-C2

	X	Y	Z
C	2.953448	1.605512	0.079413
C	1.631301	2.009865	0.103577
C	1.194771	3.346921	-0.139093
C	-1.160165	2.663916	-0.091259
C	-0.13449	3.666728	-0.196924
C	-2.545938	2.977957	-0.218045
C	2.437583	-0.811962	0.08283
C	3.355057	0.245085	0.033471
C	1.028548	-0.49329	0.404131
C	0.598719	1.009198	0.406824
C	-1.770845	0.284449	0.132551
C	-0.812745	1.319228	0.132905
C	-3.147931	0.62651	-0.007186
C	-3.506131	1.98996	-0.149535
C	1.755941	-3.157894	-0.120613
C	2.736774	-2.203747	-0.088199
C	0.357416	-2.833889	-0.05595
C	-0.021685	-1.492945	0.140926
C	-2.375888	-2.124167	0.014549
C	-1.382881	-1.10843	0.136107
C	-3.753	-1.733594	-0.024455
C	-4.121199	-0.409701	-0.037528
C	-0.653521	-3.823409	-0.170536
C	-1.983705	-3.480277	-0.112363
H	-0.441492	4.691683	-0.371505
H	-4.558763	2.251333	-0.246369
H	1.948097	4.117227	-0.283033
H	3.733833	2.354129	-0.020712

H	3.772684	-2.520852	-0.150479
H	2.0337	-4.203228	-0.228166
H	-0.361434	-4.862163	-0.301271
H	-2.753064	-4.239786	-0.192745
H	-5.173738	-0.140687	-0.111784
O	-2.852805	4.295084	-0.405141
O	-4.659401	-2.752641	-0.08592
O	5.67043	0.697936	0.417558
O	5.21965	-0.873611	-1.09167
O	0.827586	0.258551	1.607934
C	4.835207	0.051176	-0.165653
H	-3.815535	4.388416	-0.477032
H	-5.552792	-2.377758	-0.132279
H	4.436974	-1.200067	-1.56639

E= -1335.9976363 (Hartree)

O-A-C2

	X	Y	Z
C	2.941804	1.624718	0.068696
C	1.614595	2.016531	0.080294
C	1.167588	3.33856	-0.207403
C	-1.194789	2.652572	-0.105672
C	-0.165589	3.645258	-0.264942
C	-2.59198	2.971019	-0.190692
C	2.447534	-0.795741	0.090762
C	3.356937	0.269474	0.040651
C	1.034912	-0.488635	0.404284
C	0.58822	1.015535	0.396718
C	-1.770838	0.264294	0.127751
C	-0.827738	1.31168	0.123599
C	-3.151506	0.59371	-0.012771
C	-3.52735	1.951299	-0.125403
C	1.787471	-3.147596	-0.110493
C	2.75998	-2.184514	-0.07566
C	0.386599	-2.836127	-0.052235
C	-0.005175	-1.497682	0.142768
C	-2.35235	-2.1504	0.008804

C	-1.369523	-1.124449	0.132717
C	-3.733142	-1.773127	-0.034383
C	-4.113838	-0.45338	-0.045968
C	-0.614654	-3.83497	-0.170066
C	-1.947821	-3.502751	-0.116956
H	-0.454397	4.66052	-0.517625
H	-4.58586	2.195912	-0.190421
H	1.912325	4.106887	-0.39848
H	3.714554	2.380133	-0.039835
H	3.798852	-2.492756	-0.132772
H	2.075125	-4.190618	-0.215294
H	-0.312727	-4.871069	-0.299715
H	-2.71058	-4.268628	-0.200312
H	-5.16889	-0.194288	-0.120928
O	-4.629894	-2.801109	-0.100098
O	5.665698	0.746503	0.435931
O	5.238805	-0.837719	-1.066889
O	0.824613	0.273752	1.599316
C	4.839853	0.088435	-0.148199
H	-5.525904	-2.433406	-0.15289
H	4.461946	-1.174264	-1.544166
N	-2.988481	4.295986	-0.389883
H	-3.981791	4.449557	-0.26303
H	-2.452254	4.986432	0.121374

E= -1316.1337295 (Hartree)

DOX/A-C2

	X	Y	Z
C	-6.55652	-3.53434	1.002816
C	-5.372517	-2.749335	0.915096
C	-4.158865	-3.127332	1.548125
C	-3.014172	-1.150016	0.686595
C	-3.026599	-2.357812	1.442097
C	-1.82852	-0.338533	0.534365
C	-7.792938	-1.912503	-0.32828
C	-7.722333	-3.133387	0.401923
C	-6.623937	-1.110951	-0.4336

C	-5.40646	-1.530272	0.183409
C	-4.29232	0.500877	-0.653761
C	-4.227761	-0.726422	0.071244
C	-3.122866	1.304056	-0.754714
C	-1.920988	0.862137	-0.15969
C	-9.072271	-0.271818	-1.621162
C	-8.997927	-1.461139	-0.924298
C	-7.895067	0.541355	-1.77397
C	-6.684167	0.116913	-1.159737
C	-5.550425	2.145873	-1.993429
C	-5.508573	0.922318	-1.268155
C	-4.366098	2.933466	-2.078226
C	-3.200379	2.530882	-1.481267
C	-7.89627	1.753908	-2.518941
C	-6.765858	2.528301	-2.618669
H	-1.027636	1.471109	-0.267202
H	-4.139884	-4.041744	2.137153
H	-6.522706	-4.466221	1.56301
H	-8.617556	-3.746054	0.481618
H	-9.893041	-2.070763	-0.811314
H	-8.793811	2.059303	-3.047726
H	-6.788128	3.449842	-3.196104
H	-4.401716	3.868118	-2.633711
H	-2.305645	3.144393	-1.560507
N	-10.26934	0.133307	-2.230426
H	-10.45411	1.1277	-2.165152
H	-11.07564	-0.392474	-1.912643
H	-2.138413	-2.675547	1.976934
N	-0.60013	-0.751947	1.014064
H	-0.551456	-1.557869	1.621311
H	0.061576	-0.016714	1.249085
C	1.438095	6.987297	1.373381
C	2.332462	6.343974	0.523442
C	2.431497	4.949348	0.548201
C	1.612895	4.171813	1.397307
C	0.722581	4.840729	2.267309
C	0.651378	6.239392	2.247051
H	1.363375	8.07107	1.369097
H	2.970623	6.897503	-0.155966
H	-0.024012	6.723294	2.946367
C	3.683996	2.864051	-0.176536

C	4.732755	2.272944	-0.907858
C	5.035762	0.899612	-0.737089
C	4.309853	0.154734	0.184479
C	3.206302	0.722962	0.886276
C	2.885891	2.075497	0.701837
C	1.673609	2.680041	1.322424
C	3.438048	4.3022	-0.326722
C	6.159102	0.318844	-1.563845
C	6.16963	-1.221674	-1.595995
C	5.982948	-1.747031	-0.159864
C	4.645744	-1.299641	0.431083
H	7.124598	0.673503	-1.180657
H	6.036194	-2.842256	-0.141909
O	-0.005945	4.176087	3.211123
O	4.088962	4.991476	-1.137196
O	0.726681	1.998274	1.705525
O	2.49868	0.003598	1.784201
O	5.489074	2.956788	-1.780796
H	2.587198	-0.963269	1.662852
H	5.141694	3.891381	-1.779306
C	-1.366374	3.876474	2.870568
H	-1.811198	3.449924	3.771482
H	-1.910395	4.788772	2.592163
H	-1.409732	3.145337	2.059313
O	8.568697	-1.34104	-1.594287
C	7.526954	-1.704467	-2.117714
C	7.572324	-2.665964	-3.291844
H	6.953781	-3.543731	-3.049998
H	7.076583	-2.182877	-4.149038
O	8.890646	-3.035778	-3.590482
H	9.450238	-2.522367	-2.975882
O	5.17498	-1.738985	-2.474543
H	4.346773	-1.842871	-1.974099
O	3.5436	-2.060228	-0.165655
C	3.153167	-3.223211	0.511581
C	2.007105	-3.86167	-0.257314
C	1.437324	-5.052526	0.526401
H	1.233292	-3.097619	-0.391042
C	2.248903	-3.891426	2.641151
C	1.078683	-4.622113	1.971406
O	2.722242	-2.817693	1.806204

O	-0.064267	-3.790896	1.942482
N	0.19435	-5.508088	-0.109037
C	1.904433	-3.290596	3.994913
H	2.775731	-2.778804	4.414152
H	1.084757	-2.575063	3.897075
H	1.595761	-4.079148	4.688977
H	-0.030074	-6.462425	0.166497
H	0.268563	-5.495646	-1.123672
H	-0.583623	-4.123637	1.17728
H	2.35862	-4.180962	-1.24595
H	4.003448	-3.919332	0.632975
H	2.205528	-5.842644	0.585048
H	0.87655	-5.529674	2.569377
H	3.070421	-4.619291	2.754138
H	6.079462	0.694918	-2.588738
H	4.642674	-1.497078	1.507905
H	6.802962	-1.370737	0.4612

E= -2961.1364089 (Hartree)

DOX/A-C3

	X	Y	Z
C	4.692873	-3.649533	-1.022062
C	3.448247	-3.809631	-0.403844
C	3.031561	-5.057864	0.173607
C	0.889947	-4.095884	0.846339
C	1.812844	-5.194559	0.766528
C	-0.368342	-4.217647	1.444794
C	6.717948	-1.067847	-2.785184
C	6.36057	-2.255651	-2.219066
C	4.19698	-1.309973	-1.54338
C	5.085057	-2.43043	-1.590772
C	2.931778	-1.449301	-0.908549
C	2.550991	-2.696282	-0.341998
C	0.390555	-1.729886	0.355127
C	1.27881	-2.837247	0.286725
C	-0.877326	-1.868915	0.983855
C	-1.259211	-3.13807	1.522536

C	-3.408595	-2.194097	2.183978
C	-2.562124	-3.260658	2.105272
C	6.184875	1.296357	-3.404044
C	5.83986	0.06897	-2.782583
C	3.681589	1.040936	-2.065537
C	4.576259	-0.060868	-2.126173
C	2.415577	0.905301	-1.418523
C	2.035132	-0.338428	-0.84876
C	-0.116116	0.630091	-0.143587
C	0.774321	-0.474668	-0.209431
C	-1.381739	0.494797	0.503557
C	-1.765768	-0.751728	1.067352
C	-3.907846	0.223386	1.820544
C	-3.035622	-0.895267	1.701719
C	5.674917	3.708728	-3.824929
C	5.32676	2.419906	-3.29416
C	3.171986	3.398378	-2.561654
C	4.064929	2.284613	-2.634935
C	1.908212	3.2624	-1.923112
C	1.525117	2.008956	-1.354729
C	-0.626887	2.986962	-0.642306
C	0.265325	1.873791	-0.712194
C	-1.885449	2.851605	0.008023
C	-2.272141	1.599008	0.581158
C	-4.358889	2.642914	1.348387
C	-3.530821	1.472678	1.254058
C	4.827843	4.773971	-3.744669
C	2.653037	5.740965	-3.043974
C	3.541501	4.660931	-3.124039
C	1.403928	5.625703	-2.424041
C	1.020243	4.370333	-1.853609
C	-1.134791	5.351943	-1.133658
C	-0.24574	4.233517	-1.210775
C	-2.36552	5.201171	-0.485713
C	-2.755522	3.984324	0.08881
C	-3.997064	3.831635	0.78605
C	0.486384	6.727471	-2.334872
C	-0.722411	6.596962	-1.720268
H	-5.296469	2.601938	1.891458
H	-4.400543	-2.329961	2.597865
H	-2.874788	-4.23493	2.473636

H	-0.666786	-5.178087	1.860225
H	1.514695	-6.148641	1.194792
H	3.716	-5.901496	0.124117
H	5.37577	-4.495647	-1.065452
H	7.052091	-3.094669	-2.22982
H	7.713343	-0.978107	-3.209615
H	6.654678	3.862414	-4.267257
H	5.125631	5.739123	-4.147226
H	2.944368	6.696816	-3.474758
H	0.780908	7.679019	-2.771228
H	-1.401978	7.443905	-1.660173
H	-3.036544	6.05521	-0.417513
H	-4.648063	4.697732	0.879734
N	-5.130135	0.040763	2.45575
H	-5.759473	0.832656	2.484276
H	-5.097002	-0.446688	3.349617
N	7.399689	1.412545	-4.087455
H	7.404706	2.123865	-4.806518
H	7.749101	0.541409	-4.464597
C	-1.439349	-3.942808	8.364051
C	-2.371581	-4.773385	7.749963
C	-3.366372	-4.219167	6.93839
C	-3.426359	-2.827764	6.698768
C	-2.476038	-1.997391	7.33505
C	-1.501578	-2.565304	8.165331
H	-0.671024	-4.364044	9.006195
H	-2.356924	-5.848013	7.891966
H	-0.804338	-1.895315	8.659514
C	-5.529304	-4.552978	5.653251
C	-6.554328	-5.408738	5.204456
C	-7.71564	-4.872483	4.595108
C	-7.849518	-3.493317	4.487785
C	-6.797777	-2.617853	4.888045
C	-5.629183	-3.145754	5.455636
C	-4.4544	-2.27989	5.762482
C	-4.371332	-5.131569	6.34304
C	-8.766816	-5.841363	4.105983
C	-9.782636	-5.209436	3.133994
C	-10.26059	-3.869055	3.723882
C	-9.102338	-2.88618	3.895681
H	-9.309239	-6.265899	4.960493

H	-11.02371	-3.416126	3.079654
O	-2.524271	-0.63569	7.249803
O	-4.24513	-6.365495	6.475259
O	-4.298767	-1.185329	5.228684
O	-6.922029	-1.276377	4.791439
O	-6.494778	-6.744191	5.327229
H	-7.622346	-0.993959	4.169111
H	-5.625159	-6.94519	5.771838
C	-1.69505	-0.041449	6.241662
H	-1.815285	1.037382	6.355661
H	-0.641657	-0.310581	6.394917
H	-2.023356	-0.34462	5.244638
O	-11.60725	-6.522506	3.979723
C	-10.99272	-6.13923	2.99653
C	-11.44439	-6.572209	1.613024
H	-11.61767	-5.672466	1.003095
H	-10.60682	-7.099786	1.12913
O	-12.59397	-7.370451	1.684581
H	-12.77475	-7.481292	2.638239
O	-9.233529	-5.040667	1.830721
H	-8.791234	-4.174796	1.792093
O	-8.693668	-2.34362	2.596629
C	-9.300369	-1.142626	2.204702
C	-8.733674	-0.738487	0.852045
C	-9.243243	0.65438	0.455324
H	-7.64181	-0.727485	0.941486
C	-9.48525	1.144883	2.940467
C	-8.977953	1.672382	1.593612
O	-8.968207	-0.17472	3.195334
O	-7.592695	1.948785	1.666168
N	-8.510697	1.129613	-0.725932
C	-9.102039	2.016361	4.126228
H	-9.490951	1.586411	5.053997
H	-8.01544	2.100947	4.201025
H	-9.520619	3.020807	4.005113
H	-9.032615	1.855523	-1.213453
H	-8.347679	0.376726	-1.390576
H	-7.289884	1.888561	0.733026
H	-9.016325	-1.482263	0.097157
H	-10.40111	-1.242342	2.176047
H	-10.33331	0.601812	0.291763

H	-9.540059	2.598519	1.374167
H	-10.58374	1.069456	2.871206
H	-8.2734	-6.682008	3.607891
H	-9.431883	-2.048716	4.51886
H	-10.72664	-4.060765	4.696415

E= -4108.1827921 (Hartree)

DOX/A-C4

	X	Y	Z
C	-8.265826	-6.858264	0.698539
C	-7.949672	-8.189029	0.659781
C	-6.929621	-2.084287	0.888863
C	-6.607236	-3.463457	0.864763
C	-7.594746	-4.476277	0.81754
C	-5.885583	-6.218858	0.807272
C	-7.269535	-5.829049	0.786521
C	-5.537847	-7.596098	0.780589
C	-6.555176	-8.613275	0.728037
C	-4.826985	-10.35953	0.780752
C	-6.183528	-9.951561	0.749985
C	-4.446061	-11.72281	0.784159
C	-5.301542	1.262394	0.981935
C	-6.271259	0.310559	0.947885
C	-4.564352	-1.47291	0.947884
C	-5.952105	-1.096741	0.927849
C	-4.213508	-2.84898	0.929287
C	-5.226651	-3.845475	0.884834
C	-3.500136	-5.607544	0.880405
C	-4.875096	-5.224291	0.861465
C	-3.148655	-6.980492	0.865637
C	-4.168757	-7.979956	0.813937
C	-2.437167	-9.740317	0.837158
C	-3.807048	-9.356299	0.808204
C	-2.080498	-11.11512	0.833477
C	-3.112802	-12.11592	0.805661
C	-1.403615	-13.86667	0.820515
C	-2.712882	-13.50228	0.800353

C	-2.894594	1.875357	1.034036
C	-3.900587	0.916668	1.00174
C	-2.181972	-0.856145	1.005453
C	-3.550575	-0.478342	0.985692
C	-1.826881	-2.239153	0.99231
C	-2.838053	-3.231013	0.946864
C	-1.116974	-4.991141	0.949494
C	-2.48437	-4.610358	0.9324
C	-0.762826	-6.369982	0.94041
C	-1.776344	-7.363205	0.887799
C	-0.053318	-9.121938	0.903233
C	-1.418552	-8.741475	0.879036
C	0.303364	-10.50462	0.894825
C	-0.711845	-11.49658	0.858636
C	0.999248	-13.24051	0.874415
C	-0.344788	-12.88704	0.850818
C	-0.489153	2.494667	1.08414
C	-1.522169	1.526264	1.053969
C	0.205374	-0.241698	1.063876
C	-1.165389	0.138301	1.042143
C	0.561404	-1.624519	1.056225
C	-0.455189	-2.620312	1.010942
C	1.270593	-4.376786	1.021998
C	-0.10091	-3.995071	1.002567
C	1.624747	-5.755541	1.014859
C	0.608806	-6.75156	0.959671
C	2.335013	-8.50739	0.974896
C	0.963238	-8.126256	0.951482
C	2.690362	-9.890201	0.963131
C	1.67423	-10.88455	0.920799
C	3.403845	-12.62147	0.936404
C	2.031689	-12.27226	0.909398
C	1.915108	3.120438	1.13378
C	0.85513	2.141161	1.104246
C	2.589469	0.368463	1.12071
C	1.221004	0.750176	1.096809
C	2.945185	-1.00663	1.12075
C	1.926373	-2.005235	1.080409
C	3.656311	-3.766476	1.104157
C	2.284072	-3.383666	1.07525
C	4.00795	-5.13928	1.094954

C	2.992223	-6.136269	1.037643
C	4.721689	-7.897279	1.053721
C	3.345985	-7.515614	1.026018
C	5.072242	-9.273527	1.03778
C	4.059051	-10.26788	0.991293
C	5.810193	-12.00845	1.006998
C	4.409376	-11.66292	0.976467
C	3.224823	2.756688	1.152561
C	4.954631	0.973747	1.166322
C	3.622183	1.369165	1.145762
C	5.334978	-0.389807	1.180306
C	4.314368	-1.391508	1.155026
C	6.045073	-3.150646	1.209731
C	4.676112	-2.767397	1.160082
C	6.392887	-4.527686	1.189945
C	5.383072	-5.522092	1.126017
C	7.115332	-7.281267	1.144068
C	5.734087	-6.901009	1.107577
C	7.436932	-8.66137	1.121865
C	6.46003	-9.649001	1.070733
C	6.779261	-11.05636	1.051362
C	6.691001	-0.797226	1.226846
C	8.46151	-2.549083	1.366199
C	7.062153	-2.134283	1.27184
C	8.773353	-3.886584	1.334426
C	7.7788	-4.913373	1.230544
C	8.101701	-6.268796	1.204667
H	4.004768	3.514393	1.178775
H	5.733726	1.732696	1.17683
H	7.456245	-0.029901	1.217883
H	9.812454	-4.190353	1.439043
H	9.148506	-6.563921	1.240414
H	8.484939	-8.953352	1.149985
H	7.827928	-11.34358	1.075393
H	-3.492676	-14.25988	0.779577
H	-5.224122	-12.48335	0.766534
H	-6.943197	-10.72732	0.775849
H	-9.309592	-6.55483	0.641169
H	-8.642039	-4.181917	0.799075
H	-7.977844	-1.792794	0.873135
H	-7.319979	0.597821	0.933315

H	-5.568894	2.316336	0.995289
H	-3.165574	2.92906	1.044748
H	-0.76136	3.548076	1.091504
H	1.63959	4.172296	1.140821
H	6.077823	-13.06233	0.994428
H	3.674731	-13.67515	0.926258
H	1.271408	-14.29389	0.867009
H	-1.127752	-14.91843	0.815212
N	9.439962	-1.565322	1.429011
N	-8.938277	-9.178323	0.609206
H	-9.861869	-8.8132	0.405901
H	-8.7224	-9.953232	-0.007898
H	9.261622	-0.789223	2.064235
H	10.384714	-1.927343	1.524755
C	5.378394	3.904982	5.755428
C	5.779	4.419816	4.526181
C	6.783676	3.774757	3.798294
C	7.379245	2.583061	4.27015
C	6.964305	2.0757	5.521341
C	5.976953	2.748868	6.251631
H	4.608318	4.407712	6.333469
H	5.338872	5.32228	4.117511
H	5.701957	2.347916	7.222616
C	8.422531	3.847907	1.863779
C	8.946524	4.522962	0.743576
C	10.142846	4.070496	0.132912
C	10.801307	2.969973	0.668085
C	10.251336	2.239732	1.762305
C	9.058441	2.671987	2.357604
C	8.3855	1.874506	3.422485
C	7.22323	4.380285	2.518932
C	10.653525	4.832632	-1.068309
C	11.718168	4.070357	-1.881369
C	12.749355	3.466806	-0.90828
C	12.09751	2.48048	0.060115
H	11.073675	5.793482	-0.743872
H	13.544163	2.954525	-1.46359
O	7.562738	0.992918	6.09883
O	6.600282	5.352172	2.043969
O	8.592228	0.67215	3.56406
O	10.894825	1.177649	2.291968

O	8.364016	5.607409	0.208691
H	11.516828	0.750873	1.668069
H	7.540198	5.776124	0.743569
C	6.903041	-0.265196	5.901754
H	7.477697	-0.995277	6.474633
H	5.873488	-0.230261	6.281513
H	6.908109	-0.540277	4.844055
O	12.973243	6.060776	-2.361491
C	12.443452	5.054284	-2.805828
C	12.519627	4.759635	-4.293219
H	12.955497	3.758263	-4.430444
H	11.490635	4.68904	-4.680875
O	13.265414	5.73831	-4.963839
H	13.50259	6.396981	-4.282489
O	11.134537	3.070728	-2.710806
H	11.043245	2.254547	-2.188643
O	11.750133	1.238204	-0.635404
C	12.700164	0.210623	-0.597065
C	12.164217	-0.960297	-1.406881
C	13.078175	-2.184826	-1.256027
H	11.162642	-1.188412	-1.026309
C	13.778557	-1.236838	0.998682
C	13.329452	-2.492338	0.242166
O	12.855465	-0.154895	0.771153
O	12.149068	-3.015893	0.820535
N	12.417361	-3.36381	-1.83222
C	13.887611	-1.430678	2.50309
H	14.201669	-0.498974	2.982815
H	12.926235	-1.739175	2.920593
H	14.627587	-2.205493	2.728832
H	13.095379	-4.090227	-2.055546
H	11.929066	-3.131594	-2.694194
H	11.721622	-3.502854	0.081269
H	12.079194	-0.669582	-2.461033
H	13.680087	0.557759	-0.973377
H	14.05109	-1.964502	-1.72752
H	14.149225	-3.229783	0.317215
H	14.758546	-0.938077	0.589158
H	9.811243	5.072664	-1.724896
H	12.805791	2.232861	0.857522
H	13.217135	4.280152	-0.343053

E= -5712.6471891 (Hartree)

DOX/O-C2

	X	Y	Z
C	1.917886	2.641478	-0.296451
C	3.211024	2.679723	0.202952
C	3.628913	3.504626	1.289961
C	5.858751	2.483626	1.308012
C	4.900085	3.438837	1.794689
C	7.165504	2.36139	1.867245
C	2.279351	0.580714	-1.61038
C	1.455749	1.616159	-1.157138
C	3.732807	0.71243	-1.408104
C	4.232359	1.833753	-0.426018
C	6.379679	0.589237	-0.187443
C	5.519425	1.620418	0.249611
C	7.676243	0.486742	0.396247
C	8.05154	1.41231	1.402076
C	2.703837	-1.590761	-2.653618
C	1.837241	-0.592202	-2.299272
C	4.094247	-1.573483	-2.284496
C	4.602487	-0.459972	-1.58844
C	6.786614	-1.535203	-1.415363
C	5.929712	-0.440925	-1.097707
C	8.117947	-1.535616	-0.889367
C	8.542191	-0.563937	-0.015133
C	4.973849	-2.645893	-2.588509
C	6.289771	-2.613859	-2.190059
H	5.196366	4.08549	2.612947
H	9.04532	1.339326	1.841579
H	2.907373	4.196475	1.717266
H	1.187367	3.356232	0.074057
H	0.785484	-0.686341	-2.54788
H	2.330485	-2.456896	-3.193884
H	4.592691	-3.496284	-3.14823
H	6.959211	-3.431259	-2.433376
H	9.544765	-0.615141	0.407167
O	7.477972	3.232674	2.872731

O	8.912811	-2.577647	-1.276652
O	-0.46426	2.612821	-2.156915
O	-0.789295	0.656837	-1.159769
O	4.313441	1.943678	-1.851749
C	-0.003376	1.677209	-1.533181
H	8.38405	3.056694	3.170535
H	9.777779	-2.488051	-0.847112
H	-0.370882	0.061944	-0.485504
C	0.763108	-6.222859	1.516933
C	-0.505027	-6.030159	0.975272
C	-0.996777	-4.732583	0.807731
C	-0.209715	-3.607737	1.140986
C	1.063698	-3.818561	1.710918
C	1.532833	-5.124865	1.896779
H	1.146124	-7.22884	1.663543
H	-1.135239	-6.865084	0.690269
H	2.504296	-5.257714	2.363569
C	-2.975828	-3.220196	0.349471
C	-4.342714	-3.066273	0.05301
C	-4.965954	-1.799319	0.192628
C	-4.221784	-0.724669	0.662562
C	-2.821522	-0.848769	0.905159
C	-2.194968	-2.087994	0.724306
C	-0.722515	-2.24372	0.822635
C	-2.37932	-4.557314	0.29746
C	-6.432466	-1.69465	-0.155389
C	-6.930031	-0.243855	-0.308647
C	-6.401247	0.587731	0.876573
C	-4.872564	0.620937	0.896468
H	-7.033265	-2.198915	0.612364
H	-6.781943	1.614752	0.825214
O	1.807407	-2.778926	2.188297
O	-3.026191	-5.546751	-0.099868
O	0.064208	-1.324663	0.579819
O	-2.092759	0.173773	1.39477
O	-5.116653	-4.083531	-0.356162
H	-2.450169	1.057837	1.163401
H	-4.527667	-4.886209	-0.394641
C	2.89261	-2.346584	1.356994
H	3.407503	-1.56582	1.919455
H	3.589169	-3.170715	1.155009

H	2.512443	-1.937676	0.418122
O	-9.072758	-0.753004	0.653441
C	-8.461454	-0.228306	-0.264564
C	-9.22816	0.474241	-1.371088
H	-8.861087	1.508954	-1.450562
H	-8.96562	-0.006078	-2.327112
O	-10.60844	0.43779	-1.129324
H	-10.71403	-0.086012	-0.311375
O	-6.540395	0.317246	-1.557572
H	-5.670953	0.742421	-1.447916
O	-4.369379	1.491695	-0.164031
C	-4.123888	2.82532	0.199953
C	-3.634718	3.581154	-1.024599
C	-3.182726	4.996245	-0.631724
H	-2.795585	3.02978	-1.462422
C	-2.726709	4.09027	1.695155
C	-2.175763	4.944338	0.544853
O	-3.125024	2.791701	1.212484
O	-0.940023	4.421882	0.116911
N	-2.499191	5.620461	-1.768041
C	-1.73025	3.861467	2.82031
H	-2.177634	3.24596	3.60671
H	-0.839942	3.358495	2.436003
H	-1.429127	4.819965	3.256078
H	-2.479439	6.63385	-1.673638
H	-2.962006	5.401738	-2.646761
H	-0.895568	4.583838	-0.849099
H	-4.442089	3.632394	-1.766125
H	-5.031698	3.288498	0.630288
H	-4.064435	5.567702	-0.289233
H	-2.04767	5.972042	0.935643
H	-3.626353	4.594976	2.087592
H	-6.616765	-2.232634	-1.090934
H	-4.529423	1.024701	1.854287
H	-6.772755	0.147205	1.808185

E= -3264.5407306 (Hartree)

DOX/O-A-C2

	X	Y	Z
C	-3.505056	0.837271	-1.41392
C	-2.169544	0.852495	-1.785793
C	-1.573534	-0.077324	-2.684293
C	0.586985	1.104011	-2.604006
C	-0.254559	0.025171	-3.041712
C	1.969041	1.208747	-2.986204
C	-3.477481	3.1128	-0.441436
C	-4.149427	1.927792	-0.779761
C	-2.002485	3.101015	-0.497158
C	-1.299035	1.885313	-1.214922
C	0.752557	3.275229	-1.441629
C	0.042729	2.105034	-1.775079
C	2.10344	3.395383	-1.885907
C	2.689227	2.333806	-2.609556
C	-3.338588	5.458236	0.247389
C	-4.078133	4.327867	0.017605
C	-1.928375	5.528246	-0.013374
C	-1.257495	4.367823	-0.447961
C	0.83305	5.614908	-0.603662
C	0.113394	4.398618	-0.79573
C	2.214162	5.656934	-0.980372
C	2.821187	4.58925	-1.595752
C	-1.184755	6.724076	0.165788
C	0.164414	6.757593	-0.098167
H	0.149961	-0.702231	-3.73796
H	3.733353	2.416604	-2.904488
H	-2.179414	-0.888395	-3.075786
H	-4.125422	0.000513	-1.723014
H	-5.143248	4.352053	0.225626
H	-3.834915	6.352901	0.614855
H	-1.696546	7.614881	0.520978
H	0.731653	7.669894	0.047829
H	3.861905	4.663935	-1.907692
O	2.866479	6.829194	-0.722954
O	-6.103726	0.760416	-0.04351
O	-6.443988	2.733674	-0.998775
O	-1.3817	2.02061	0.207456

C	-5.62194	1.747141	-0.560701
H	3.779032	6.756652	-1.043758
H	-5.921545	3.393747	-1.486029
N	2.553347	0.214547	-3.76172
H	3.565758	0.248333	-3.786637
H	2.241056	-0.733157	-3.582551
C	7.658698	-0.419607	0.466505
C	6.694246	-0.85619	-0.434554
C	5.385322	-1.084873	0.005726
C	5.005569	-0.851116	1.345844
C	6.002579	-0.418942	2.251364
C	7.313087	-0.215473	1.80059
H	8.680606	-0.252656	0.137739
H	6.932051	-1.044524	-1.475253
H	8.054779	0.092023	2.531787
C	3.095627	-2.058544	-0.491533
C	2.229566	-2.707981	-1.393322
C	0.98469	-3.214702	-0.958683
C	0.611602	-3.025432	0.365986
C	1.433254	-2.292478	1.274733
C	2.696311	-1.837469	0.859115
C	3.579203	-1.049702	1.771644
C	4.409093	-1.618778	-0.968226
C	0.148475	-3.987274	-1.955138
C	-1.297886	-4.268723	-1.50085
C	-1.294266	-4.670653	-0.011384
C	-0.710688	-3.562575	0.865263
H	0.643842	-4.943117	-2.168467
H	-2.314486	-4.895196	0.321559
O	5.777567	-0.27582	3.590985
O	4.734751	-1.725711	-2.173085
O	3.166695	-0.554409	2.810873
O	1.052686	-2.111943	2.551837
O	2.54103	-2.883342	-2.698503
H	0.078089	-2.065179	2.664403
H	3.47435	-2.539028	-2.800025
C	5.366484	1.024507	4.029036
H	5.295773	0.962582	5.116639
H	6.1139	1.781236	3.753823
H	4.389423	1.280283	3.613136
O	-1.255174	-6.494699	-2.407923

C	-1.864578	-5.441212	-2.309818
C	-3.22119	-5.296072	-2.976648
H	-3.957415	-4.994559	-2.215903
H	-3.165353	-4.453532	-3.684089
O	-3.600035	-6.485846	-3.613069
H	-2.848769	-7.097711	-3.487768
O	-2.154168	-3.153597	-1.731454
H	-2.080424	-2.554974	-0.964551
O	-1.618196	-2.418236	0.89551
C	-2.496493	-2.355006	1.989498
C	-3.459401	-1.201409	1.777548
C	-4.344651	-1.021811	3.018659
H	-2.871803	-0.294302	1.602607
C	-2.430632	-2.020295	4.375059
C	-3.463473	-0.887946	4.28648
O	-1.691497	-2.142871	3.141583
O	-2.810866	0.359679	4.279289
N	-5.120939	0.215634	2.886251
C	-1.408136	-1.822775	5.483
H	-0.688248	-2.647027	5.488244
H	-0.875726	-0.880945	5.3328
H	-1.909505	-1.789731	6.45601
H	-5.927902	0.199519	3.507706
H	-5.472444	0.328077	1.934615
H	-3.446004	0.950723	3.820464
H	-4.077393	-1.386355	0.89207
H	-3.033493	-3.314229	2.11304
H	-4.978069	-1.919618	3.133267
H	-4.117056	-0.984712	5.175823
H	-2.982931	-2.962984	4.531452
H	0.113901	-3.443528	-2.904349
H	-0.59095	-3.930832	1.889109
H	-0.699234	-5.582919	0.10746

E= -3244.6703471 (Hartree)

Cartesian coordinates (Å) for the studied compounds in aqueous

DOX

	X	Y	Z
C	7.149511	-0.776444	-0.127219
C	6.064313	-1.597631	-0.417798
C	4.763737	-1.088787	-0.336549
C	4.523569	0.261537	0.003438
C	5.636673	1.074989	0.312836
C	6.931964	0.547522	0.248404
H	8.161099	-1.167754	-0.176206
H	6.203021	-2.636722	-0.693063
H	7.762062	1.19535	0.513433
C	2.27126	-1.553683	-0.301521
C	1.216895	-2.484958	-0.365789
C	-0.099617	-2.104324	-0.008306
C	-0.340652	-0.796345	0.391276
C	0.699017	0.182777	0.377419
C	2.012539	-0.195463	0.052223
C	3.124135	0.797892	0.002246
C	3.633623	-2.01181	-0.58347
C	-1.16822	-3.172683	-0.041889
C	-2.604056	-2.629919	0.081921
C	-2.637602	-1.558627	1.190791
C	-1.722475	-0.38317	0.850245
H	-0.985955	-3.889632	0.768604
H	-3.656949	-1.186132	1.339879
O	5.494551	2.358846	0.769921
O	3.860961	-3.176711	-0.976862
O	2.919363	2.006536	-0.068711
O	0.456425	1.454906	0.754758
O	1.399185	-3.765231	-0.736259
H	-0.489314	1.71346	0.679511
H	2.371291	-3.855357	-0.944183
C	5.657299	3.385082	-0.219425
H	5.590776	4.3343	0.315712
H	6.637242	3.308651	-0.706011
H	4.859891	3.32537	-0.965399
O	-3.29815	-4.506463	1.424498
C	-3.547088	-3.767704	0.482545
C	-4.834461	-3.965661	-0.297469
H	-5.397143	-3.020884	-0.297483

H	-4.571619	-4.163633	-1.347489
O	-5.595455	-5.01499	0.251963
H	-5.054444	-5.361941	0.9892
O	-3.06688	-2.113257	-1.164196
H	-2.932032	-1.147096	-1.161663
O	-2.311271	0.40158	-0.236943
C	-3.064758	1.515005	0.173419
C	-3.857035	2.051734	-1.006049
C	-4.553153	3.366351	-0.62162
H	-3.162185	2.228761	-1.833773
C	-2.707666	3.713794	1.094272
C	-3.532093	4.364058	-0.023228
O	-2.118333	2.48077	0.625539
O	-2.675791	4.834004	-1.051906
N	-5.115119	3.993785	-1.828554
C	-1.572281	4.584732	1.607539
H	-1.021079	4.063439	2.396221
H	-0.885017	4.831196	0.794013
H	-1.972305	5.515742	2.021791
H	-5.819465	4.682491	-1.565438
H	-5.595389	3.299388	-2.398697
H	-3.261845	4.845495	-1.840047
H	-4.593418	1.305153	-1.324125
H	-3.725705	1.249739	1.014472
H	-5.31651	3.154445	0.143391
H	-4.088182	5.203694	0.42976
H	-3.395869	3.471357	1.918914
H	-1.086302	-3.737984	-0.975941
H	-1.633284	0.265304	1.727823
H	-2.31264	-2.012207	2.132794

E= -1928.5474387 (Hartree)

A-C2

	X	Y	Z
C	0.24411	3.739985	-0.03046
C	-0.77348	2.743481	-0.02584
C	-2.15695	3.066517	-0.04925
C	-2.77118	0.704713	0.002143
C	-3.1201	2.086227	-0.03824

C	-3.76027	-0.34329	0.035247
C	1.987792	2.03565	-0.00608
C	1.573126	3.400362	-0.0186
C	0.991663	1.02136	-0.00344
C	-0.39235	1.373385	-0.00878
C	-0.99166	-1.02136	-0.00344
C	-1.39232	0.350143	0.00016
C	-1.98779	-2.03565	-0.00609
C	-3.35575	-1.66561	0.024444
C	3.760267	0.343292	0.035245
C	3.355747	1.665607	0.024444
C	2.771183	-0.70471	0.00214
C	1.39232	-0.35014	0.000157
C	0.773479	-2.74348	-0.02585
C	0.392346	-1.37339	-0.00878
C	-0.24411	-3.73999	-0.03047
C	-1.57313	-3.40036	-0.01861
C	3.120096	-2.08623	-0.03824
C	2.156949	-3.06652	-0.04925
H	-4.10709	-2.45182	0.050902
H	-2.45002	4.112707	-0.08355
H	-0.0515	4.786142	-0.04318
H	2.335201	4.175841	-0.01974
H	4.107085	2.451824	0.050899
H	4.164907	-2.3762	-0.08533
H	2.450014	-4.11271	-0.08355
H	0.0515	-4.78614	-0.04319
H	-2.3352	-4.17584	-0.01974
N	5.118377	0.008091	0.011667
H	5.369218	-0.79445	0.578641
H	5.728686	0.787721	0.232888
H	-4.16491	2.376197	-0.08533
N	-5.11838	-0.00808	0.011668
H	-5.36922	0.794398	0.578738
H	-5.72869	-0.78773	0.232824

E= -1032.6160455 (Hartree)

A-C3

	X	Y	Z
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
C	-2.82989	-4.91223	-0.02734
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C	-2.82989	-4.91223	-0.02734
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C	-2.82989	-4.91223	-0.02734
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C	-2.82989	-4.91223	-0.02734
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C	-2.82989	-4.91223	-0.02734
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C	-2.82989	-4.91223	-0.02734
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C	-2.82989	-4.91223	-0.02734

C	-2.82989	-4.91223	-0.02734
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C	-2.82989	-4.91223	-0.02734
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H	-2.82989	-4.91223	-0.02734
N	-2.82989	-4.91223	-0.02734
H	-2.82989	-4.91223	-0.02734
H	-2.82989	-4.91223	-0.02734
N	-2.82989	-4.91223	-0.02734
H	-2.82989	-4.91223	-0.02734
H	-2.82989	-4.91223	-0.02734

E= -2179.6644725 (Hartree)

A-C4

	X	Y	Z
C	8.44215	-1.9112	-0.0308
C	8.66723	-0.5589	-0.0518
C	5.36621	-5.8031	0.02918
C	5.59953	-4.4048	0.02263
C	6.90212	-3.851	0.01925
C	5.99569	-1.5834	-0.0005
C	7.12404	-2.4756	0.00645
C	6.20622	-0.1782	-0.0095
C	7.53854	0.36927	-0.0177
C	6.61225	2.64598	0.02185
C	7.70878	1.74793	0.01774
C	6.78728	4.051	0.03916
C	2.5726	-8.2663	0.02195
C	3.83509	-7.7609	0.02864
C	2.94594	-5.4558	0.01898
C	4.08243	-6.338	0.02624
C	3.15242	-4.0502	0.01666
C	4.47193	-3.5206	0.01561
C	3.55727	-1.2292	0.00084
C	4.67902	-2.1125	0.00939
C	3.76198	0.17353	0.00252
C	5.08952	0.70342	-0.0045
C	4.16813	2.99421	0.00686
C	5.28498	2.11273	0.00665
C	4.36881	4.40043	0.01856
C	5.70733	4.92704	0.03443
C	4.80476	7.20259	0.03678
C	5.87307	6.36123	0.04359
C	0.11417	-7.9052	0.00439
C	1.41247	-7.4066	0.01362
C	0.50847	-5.1075	0.00661
C	1.62657	-5.9837	0.01386
C	0.71327	-3.6943	0.00885
C	2.02951	-3.1681	0.00714
C	1.11867	-0.8805	-0.0021
C	2.23445	-1.7587	0.00838
C	1.32316	0.5285	0.00359

C	2.64225	1.05516	-0.0035
C	1.72886	3.34171	-0.0019
C	2.84276	2.46491	0.00357
C	1.93218	4.75526	0.00479
C	3.25201	5.28006	0.01444
C	2.34456	7.55057	0.01498
C	3.44914	6.70535	0.02182
C	-2.3446	-7.5506	-0.0152
C	-1.0181	-7.0529	-0.0032
C	-1.9322	-4.7552	-0.0054
C	-0.8132	-5.6342	0.00035
C	-1.7289	-3.3417	0.00106
C	-0.4063	-2.8142	-0.0001
C	-1.3232	-0.5285	-0.0046
C	-0.2039	-1.4089	0.00569
C	-1.1187	0.88048	0.0011
C	0.20386	1.40894	-0.0067
C	-0.7133	3.69428	-0.0097
C	0.40625	2.8142	-0.0008
C	-0.5085	5.10751	-0.0072
C	0.81318	5.63425	-0.0009
C	-0.1142	7.90519	-0.0046
C	1.01807	7.05291	0.00285
C	-4.8048	-7.2026	-0.0366
C	-3.4492	-6.7053	-0.022
C	-4.3688	-4.4004	-0.0188
C	-3.252	-5.28	-0.0149
C	-4.1682	-2.9942	-0.0073
C	-2.8428	-2.4649	-0.0043
C	-3.762	-0.1735	-0.0031
C	-2.6422	-1.0552	0.00269
C	-3.5573	1.22919	-0.0014
C	-2.2345	1.75867	-0.0092
C	-3.1524	4.05021	-0.017
C	-2.0295	3.16811	-0.0078
C	-2.9459	5.45579	-0.0192
C	-1.6265	5.98374	-0.0142
C	-2.5725	8.26627	-0.0217
C	-1.4124	7.40665	-0.0137
C	-5.8731	-6.3612	-0.0433
C	-6.7873	-4.0509	-0.0388

C	-5.7074	-4.927	-0.0343
C	-6.6122	-2.646	-0.0216
C	-5.285	-2.1127	-0.0068
C	-6.2063	0.17808	0.00974
C	-5.0895	-0.7034	0.00433
C	-5.9957	1.58332	0.00083
C	-4.679	2.1125	-0.0095
C	-5.5995	4.40479	-0.0222
C	-4.4719	3.5206	-0.0157
C	-5.3662	5.80322	-0.0287
C	-4.0824	6.33802	-0.026
C	-3.835	7.76095	-0.0282
C	-7.7087	-1.7479	-0.017
C	-8.6672	0.55875	0.0534
C	-7.5385	-0.3693	0.01851
C	-8.4422	1.91113	0.03235
C	-7.1241	2.47552	-0.0056
C	-6.9022	3.85103	-0.0184
H	-6.8843	-6.7594	-0.055
H	-7.7978	-4.4523	-0.0515
H	-8.7055	-2.1749	-0.0617
H	-9.2899	2.5922	0.06293
H	-7.7553	4.52563	-0.0201
H	-6.2211	6.47558	-0.033
H	-4.6922	8.42941	-0.0339
H	6.88426	6.7595	0.05564
H	7.79787	4.45239	0.05228
H	8.70562	2.17488	0.0629
H	9.28987	-2.5923	-0.0608
H	7.75522	-4.5256	0.02144
H	6.2211	-6.4755	0.03391
H	4.69229	-8.4294	0.03464
H	2.41316	-9.3415	0.02295
H	-0.0419	-8.9815	0.00339
H	-2.499	-8.6271	-0.019
H	-4.955	-8.2791	-0.0424
H	-2.4131	9.34146	-0.0225
H	0.04185	8.98146	-0.0033
H	2.49894	8.62702	0.01898
H	4.95492	8.27912	0.04276
N	-9.9588	0.0331	0.04293

N	9.95894	-0.0331	-0.0404
H	10.6778	-0.7199	-0.2421
H	10.0916	0.78746	-0.6213
H	-10.091	-0.7877	0.62366
H	-10.678	0.71977	0.24515

E= -3784.1293202 (Hartree)

O-C2

	X	Y	Z
C	2.950697	1.612401	0.06115
C	1.627498	2.013795	0.083597
C	1.187127	3.349555	-0.15926
C	-1.169006	2.662037	-0.093741
C	-0.144361	3.665157	-0.20798
C	-2.558102	2.974772	-0.210844
C	2.43989	-0.809498	0.066932
C	3.354635	0.251041	0.022992
C	1.02985	-0.489421	0.385672
C	0.59857	1.008725	0.389888
C	-1.771852	0.281334	0.132631
C	-0.816065	1.317393	0.126073
C	-3.151361	0.620889	-0.000036
C	-3.515737	1.983321	-0.138137
C	1.761411	-3.154731	-0.138463
C	2.740996	-2.198704	-0.108725
C	0.362453	-2.833574	-0.063961
C	-0.019746	-1.493192	0.133092
C	-2.374652	-2.128448	0.018287
C	-1.381693	-1.111194	0.134582
C	-3.754866	-1.740132	-0.014841
C	-4.124598	-0.415653	-0.025606
C	-0.646705	-3.825852	-0.173744
C	-1.977831	-3.483517	-0.110364
H	-0.450797	4.690165	-0.383616
H	-4.568121	2.242027	-0.228615
H	1.936818	4.121308	-0.312212
H	3.724714	2.365999	-0.05008

H	3.774984	-2.515531	-0.191581
H	2.040926	-4.197853	-0.256851
H	-0.353691	-4.863561	-0.307239
H	-2.743254	-4.24723	-0.189062
H	-5.17637	-0.148496	-0.095619
O	-2.866826	4.289266	-0.392322
O	-4.656794	-2.759161	-0.071987
O	5.658539	0.680902	0.488061
O	5.256087	-0.842285	-1.069981
O	0.835396	0.262904	1.598246
C	4.83393	0.054152	-0.143061
H	-3.830593	4.389169	-0.465751
H	-5.555475	-2.393586	-0.127915
H	4.506749	-1.15934	-1.604387

E= -1336.0197749 (Hartree)

O-A-C2

	X	Y	Z
C	2.93995	1.630929	0.055025
C	1.611771	2.020063	0.064496
C	1.161527	3.34292	-0.21379
C	-1.201	2.652445	-0.10466
C	-0.17337	3.647113	-0.26231
C	-2.60113	2.969689	-0.1897
C	2.4492	-0.79318	0.068561
C	3.356065	0.274963	0.028921
C	1.036258	-0.48511	0.381576
C	0.588337	1.014261	0.379063
C	-1.7711	0.261777	0.129097
C	-0.83047	1.310537	0.118105
C	-3.15436	0.588894	-0.00102
C	-3.53417	1.945031	-0.11553
C	1.792583	-3.14407	-0.13929
C	2.76343	-2.1786	-0.10692
C	0.390731	-2.83538	-0.06747
C	-0.00369	-1.49756	0.13013
C	-2.35179	-2.15398	0.014542

C	-1.36848	-1.12661	0.130262
C	-3.73569	-1.77883	-0.01678
C	-4.11763	-0.45849	-0.02469
C	-0.60937	-3.8369	-0.17875
C	-1.94338	-3.50523	-0.11545
H	-0.46158	4.666964	-0.49464
H	-4.59265	2.187082	-0.17786
H	1.902754	4.114859	-0.40207
H	3.706645	2.391624	-0.05892
H	3.80022	-2.48622	-0.188
H	2.081129	-4.1849	-0.25759
H	-0.30703	-4.87193	-0.31249
H	-2.70256	-4.27513	-0.19463
H	-5.17238	-0.20109	-0.09076
O	-4.62829	-2.8072	-0.07403
O	5.651011	0.717694	0.520978
O	5.275873	-0.7993	-1.04938
O	0.832926	0.273426	1.587857
C	4.837285	0.088557	-0.12288
H	-5.52967	-2.44868	-0.1289
H	4.534194	-1.12005	-1.592
N	-3.00517	4.285453	-0.4063
H	-3.9972	4.439099	-0.26353
H	-2.46693	4.993855	0.078736

E= -1316.1565319 (Hartree)

DOX/A-C2

	X	Y	Z
C	-6.55652	-3.53434	1.002816
C	-5.37252	-2.74934	0.915096
C	-4.15887	-3.12733	1.548125
C	-3.01417	-1.15002	0.686595
C	-3.0266	-2.35781	1.442097
C	-1.82852	-0.33853	0.534365
C	-7.79294	-1.9125	-0.32828
C	-7.72233	-3.13339	0.401923
C	-6.62394	-1.11095	-0.4336

C	-5.40646	-1.53027	0.183409
C	-4.29232	0.500877	-0.65376
C	-4.22776	-0.72642	0.071244
C	-3.12287	1.304056	-0.75471
C	-1.92099	0.862137	-0.15969
C	-9.07227	-0.27182	-1.62116
C	-8.99793	-1.46114	-0.9243
C	-7.89507	0.541355	-1.77397
C	-6.68417	0.116913	-1.15974
C	-5.55043	2.145873	-1.99343
C	-5.50857	0.922318	-1.26816
C	-4.3661	2.933466	-2.07823
C	-3.20038	2.530882	-1.48127
C	-7.89627	1.753908	-2.51894
C	-6.76586	2.528301	-2.61867
H	-1.02764	1.471109	-0.2672
H	-4.13988	-4.04174	2.137153
H	-6.52271	-4.46622	1.56301
H	-8.61756	-3.74605	0.481618
H	-9.89304	-2.07076	-0.81131
H	-8.79381	2.059303	-3.04773
H	-6.78813	3.449842	-3.1961
H	-4.40172	3.868118	-2.63371
H	-2.30565	3.144393	-1.56051
N	-10.2693	0.133307	-2.23043
H	-10.4541	1.1277	-2.16515
H	-11.0756	-0.39247	-1.91264
H	-2.13841	-2.67555	1.976934
N	-0.60013	-0.75195	1.014064
H	-0.55146	-1.55787	1.621311
H	0.061576	-0.01671	1.249085
C	1.438095	6.987297	1.373381
C	2.332462	6.343974	0.523442
C	2.431497	4.949348	0.548201
C	1.612895	4.171813	1.397307
C	0.722581	4.840729	2.267309
C	0.651378	6.239392	2.247051
H	1.363375	8.07107	1.369097
H	2.970623	6.897503	-0.15597
H	-0.02401	6.723294	2.946367
C	3.683996	2.864051	-0.17654

C	4.732755	2.272944	-0.90786
C	5.035762	0.899612	-0.73709
C	4.309853	0.154734	0.184479
C	3.206302	0.722962	0.886276
C	2.885891	2.075497	0.701837
C	1.673609	2.680041	1.322424
C	3.438048	4.3022	-0.32672
C	6.159102	0.318844	-1.56385
C	6.16963	-1.22167	-1.596
C	5.982948	-1.74703	-0.15986
C	4.645744	-1.29964	0.431083
H	7.124598	0.673503	-1.18066
H	6.036194	-2.84226	-0.14191
O	-0.00595	4.176087	3.211123
O	4.088962	4.991476	-1.1372
O	0.726681	1.998274	1.705525
O	2.49868	0.003598	1.784201
O	5.489074	2.956788	-1.7808
H	2.587198	-0.96327	1.662852
H	5.141694	3.891381	-1.77931
C	-1.36637	3.876474	2.870568
H	-1.8112	3.449924	3.771482
H	-1.9104	4.788772	2.592163
H	-1.40973	3.145337	2.059313
O	8.568697	-1.34104	-1.59429
C	7.526954	-1.70447	-2.11771
C	7.572324	-2.66596	-3.29184
H	6.953781	-3.54373	-3.05
H	7.076583	-2.18288	-4.14904
O	8.890646	-3.03578	-3.59048
H	9.450238	-2.52237	-2.97588
O	5.17498	-1.73899	-2.47454
H	4.346773	-1.84287	-1.9741
O	3.5436	-2.06023	-0.16566
C	3.153167	-3.22321	0.511581
C	2.007105	-3.86167	-0.25731
C	1.437324	-5.05253	0.526401
H	1.233292	-3.09762	-0.39104
C	2.248903	-3.89143	2.641151
C	1.078683	-4.62211	1.971406
O	2.722242	-2.81769	1.806204

O	-0.06427	-3.7909	1.942482
N	0.19435	-5.50809	-0.10904
C	1.904433	-3.2906	3.994913
H	2.775731	-2.7788	4.414152
H	1.084757	-2.57506	3.897075
H	1.595761	-4.07915	4.688977
H	-0.03007	-6.46243	0.166497
H	0.268563	-5.49565	-1.12367
H	-0.58362	-4.12364	1.17728
H	2.35862	-4.18096	-1.24595
H	4.003448	-3.91933	0.632975
H	2.205528	-5.84264	0.585048
H	0.87655	-5.52967	2.569377
H	3.070421	-4.61929	2.754138
H	6.079462	0.694918	-2.58874
H	4.642674	-1.49708	1.507905
H	6.802962	-1.37074	0.4612

E= -2961.1726742 (Hartree)

DOX/A-C3

	X	Y	Z
C	5.9099	-5.2974	-1.6852
C	4.56454	-4.9751	-1.4741
C	3.51175	-5.9445	-1.6154
C	1.82302	-4.2734	-1.0454
C	2.20632	-5.6099	-1.4128
C	0.48718	-3.9074	-0.8462
C	9.2849	-3.7199	-1.6478
C	8.30802	-4.6648	-1.7646
C	6.59583	-2.9984	-1.191
C	6.9279	-4.3422	-1.5533
C	5.23413	-2.6543	-0.9622
C	4.21555	-3.636	-1.1069
C	2.50215	-1.9585	-0.5208
C	2.84944	-3.2875	-0.8881
C	1.13942	-1.6084	-0.309
C	0.12363	-2.6004	-0.4894

C	-1.5773	-0.9288	0.02265
C	-1.2441	-2.2059	-0.3237
C	9.99612	-1.3596	-1.2103
C	8.98665	-2.3562	-1.3069
C	7.2702	-0.6825	-0.6915
C	7.62168	-2.0101	-1.0574
C	5.90427	-0.3382	-0.4534
C	4.88518	-1.3172	-0.5972
C	3.17651	0.35574	-0.0056
C	3.52592	-0.9728	-0.3684
C	1.80949	0.70403	0.21794
C	0.78787	-0.2728	0.06522
C	-0.9365	1.40508	0.64221
C	-0.5823	0.07766	0.2598
C	10.6513	0.97922	-0.6039
C	9.65919	-0.043	-0.7936
C	7.94102	1.62789	-0.1628
C	8.29173	0.29497	-0.5461
C	6.57994	1.97337	0.06732
C	5.55568	0.98864	-0.0861
C	3.84781	2.66769	0.51655
C	4.19625	1.33308	0.14342
C	2.48535	3.01209	0.74281
C	1.45525	2.03124	0.5825
C	-0.1992	3.72407	1.24077
C	0.08623	2.38213	0.81415
C	10.3183	2.24719	-0.2273
C	8.5935	3.92691	0.37385
C	8.95438	2.62547	-0.0022
C	7.25968	4.28644	0.59935
C	6.23359	3.30007	0.44423
C	4.52153	4.98116	1.05559
C	4.86814	3.64648	0.67148
C	3.17743	5.30004	1.28008
C	2.15779	4.34877	1.13512
C	0.78234	4.66059	1.38655
C	6.8789	5.61825	0.98451
C	5.57476	5.94896	1.20203
H	-1.2187	4.01397	1.4664
H	-2.6237	-0.6604	0.0997
H	-2.0223	-2.9445	-0.4979

H	-0.2924	-4.6546	-0.977
H	1.42425	-6.3561	-1.528
H	3.7814	-6.9604	-1.8928
H	6.17429	-6.3156	-1.9616
H	8.56859	-5.689	-2.0183
H	10.3148	-4.0292	-1.7926
H	11.7027	0.74366	-0.7318
H	11.0942	2.99495	-0.086
H	9.37226	4.67671	0.49345
H	7.66126	6.36399	1.10055
H	5.30658	6.9613	1.49365
H	2.91548	6.31267	1.57857
H	0.53053	5.6662	1.71365
N	-2.275	1.72041	0.78893
H	-2.5349	2.68799	0.94072
H	-2.8645	1.06196	1.29262
N	11.3232	-1.6884	-1.4667
H	11.9122	-0.9169	-1.7518
H	11.4613	-2.4721	-2.0913
C	-3.6942	-5.0469	4.90746
C	-4.3512	-5.0635	3.68014
C	-4.5376	-3.8714	2.9736
C	-4.038	-2.6442	3.46633
C	-3.3841	-2.644	4.71801
C	-3.226	-3.8415	5.4261
H	-3.5583	-5.967	5.46752
H	-4.7382	-5.9855	3.26208
H	-2.74	-3.8036	6.39637
C	-5.6822	-2.6557	1.0667
C	-6.542	-2.685	-0.047
C	-7.0036	-1.4774	-0.6287
C	-6.6235	-0.2639	-0.0683
C	-5.7007	-0.2169	1.0198
C	-5.2197	-1.4094	1.58162
C	-4.1796	-1.4046	2.64464
C	-5.2928	-3.9176	1.70006
C	-7.9123	-1.5784	-1.8321
C	-8.0511	-0.2552	-2.6063
C	-8.3232	0.87783	-1.5992
C	-7.1575	1.0402	-0.6242
H	-8.908	-1.9159	-1.5179

H	-8.4886	1.82916	-2.1162
O	-2.9719	-1.483	5.31611
O	-5.6307	-5.0193	1.21732
O	-3.4251	-0.4467	2.81685
O	-5.3184	0.95308	1.57197
O	-6.9721	-3.8324	-0.6012
H	-5.5179	1.74209	1.01948
H	-6.5557	-4.5681	-0.0716
C	-1.5759	-1.1802	5.17304
H	-1.4026	-0.274	5.75639
H	-0.9558	-1.9934	5.56893
H	-1.3319	-0.9966	4.12303
O	-10.34	-0.724	-3.1939
C	-9.2391	-0.3463	-3.5678
C	-9.0455	0.06702	-5.0155
H	-8.6401	1.08885	-5.0412
H	-8.2705	-0.5788	-5.455
O	-10.257	-0.0219	-5.7275
H	-10.905	-0.3736	-5.085
O	-6.8829	0.00132	-3.3841
H	-6.3362	0.65663	-2.9127
O	-6.0254	1.68238	-1.294
C	-5.9433	3.07968	-1.1473
C	-4.7444	3.57795	-1.9372
C	-4.4779	5.06192	-1.6411
H	-3.8771	2.97927	-1.6385
C	-5.6093	4.70666	0.60704
C	-4.402	5.30917	-0.1145
O	-5.7611	3.31703	0.24737
O	-3.191	4.75244	0.38639
N	-3.1726	5.44444	-2.2021
C	-5.5265	4.77472	2.12366
H	-6.423	4.33558	2.57148
H	-4.6469	4.23634	2.48661
H	-5.4537	5.81834	2.44582
H	-3.1187	6.45746	-2.3027
H	-3.0578	5.05668	-3.137
H	-2.5683	4.87058	-0.3676
H	-4.919	3.42666	-3.0082
H	-6.8795	3.56723	-1.4635
H	-5.3081	5.66265	-2.0431

H	-4.4179	6.39641	0.06825
H	-6.5037	5.24558	0.25962
H	-7.5258	-2.3466	-2.5096
H	-7.4758	1.68494	0.20042
H	-9.2364	0.64521	-1.0419

E= -4108.2233589 (Hartree)

DOX/A-C4

	X	Y	Z
C	11.7649	-3.6291	-0.7735
C	12.2787	-2.361	-0.7584
C	7.91204	-6.752	-0.6511
C	8.44917	-5.4417	-0.6196
C	9.83956	-5.186	-0.6882
C	9.45892	-2.7783	-0.5621
C	10.3589	-3.8951	-0.6643
C	9.97424	-1.4547	-0.532
C	11.3913	-1.2125	-0.6073
C	10.9989	1.20591	-0.4172
C	11.8658	0.09069	-0.5285
C	11.4798	2.53578	-0.3557
C	4.64721	-8.5392	-0.5705
C	5.98806	-8.3236	-0.6267
C	5.63324	-5.8845	-0.4893
C	6.54425	-6.9924	-0.5905
C	6.14555	-4.5604	-0.451
C	7.5474	-4.3331	-0.5186
C	7.16409	-1.8998	-0.3852
C	8.0606	-3.0062	-0.4849
C	7.67416	-0.5781	-0.343
C	9.08322	-0.352	-0.4182
C	8.69548	2.08144	-0.2569
C	9.58716	0.9779	-0.3664
C	9.20268	3.40703	-0.2034
C	10.623	3.62593	-0.2553
C	10.2478	6.039	-0.1038
C	11.1017	4.98604	-0.2009

C	2.3334	-7.6485	-0.4135
C	3.70779	-7.4484	-0.4696
C	3.33735	-5.0113	-0.3282
C	4.23183	-6.1096	-0.4282
C	3.85036	-3.6795	-0.284
C	5.24789	-3.4547	-0.3526
C	4.86806	-1.0265	-0.2125
C	5.75989	-2.1266	-0.3099
C	5.37953	0.30123	-0.1644
C	6.77958	0.52614	-0.2403
C	6.39767	2.95368	-0.0873
C	7.28775	1.85547	-0.1917
C	6.90931	4.28594	-0.0383
C	8.31042	4.50798	-0.0979
C	7.92965	6.91655	0.05437
C	8.81815	5.85254	-0.0476
C	0.01707	-6.7637	-0.2587
C	1.41915	-6.5714	-0.3139
C	1.03879	-4.1335	-0.1659
C	1.9337	-5.2346	-0.2681
C	1.55106	-2.8015	-0.1162
C	2.95529	-2.5767	-0.1848
C	2.56972	-0.1491	-0.0362
C	3.4643	-1.2523	-0.1361
C	3.08118	1.17839	0.01386
C	4.48476	1.40431	-0.0646
C	4.09858	3.83134	0.08821
C	4.99361	2.72876	-0.0157
C	4.6113	5.16311	0.1338
C	6.01438	5.38688	0.0681
C	5.61447	7.80047	0.22094
C	6.52824	6.72384	0.1143
C	-2.3021	-5.8848	-0.1047
C	-0.8717	-5.6993	-0.1603
C	-1.2547	-3.2539	-0.0053
C	-0.3627	-4.355	-0.1096
C	-0.7464	-1.9288	0.05187
C	0.66135	-1.7032	-0.0118
C	0.27548	0.7299	0.14983
C	1.16978	-0.374	0.04033
C	0.78548	2.05124	0.1975

C	2.18939	2.27819	0.11695
C	1.80358	4.71127	0.27094
C	2.7014	3.60621	0.16249
C	2.3163	6.03515	0.31192
C	3.71689	6.26084	0.24223
C	3.30157	8.68985	0.39637
C	4.24072	7.59982	0.28485
C	-3.1568	-4.832	-0.009
C	-3.5302	-2.3807	0.14332
C	-2.6754	-3.4723	0.04381
C	-3.0483	-1.0515	0.21533
C	-1.6369	-0.8253	0.16664
C	-2.0239	1.60498	0.3592
C	-1.133	0.50368	0.22915
C	-1.5086	2.92812	0.39623
C	-0.1111	3.15672	0.3093
C	-0.5002	5.58983	0.46535
C	0.40271	4.48317	0.34789
C	0.03815	6.90042	0.49872
C	1.40518	7.14188	0.42604
C	1.96136	8.47314	0.4629
C	-3.9147	0.06211	0.34231
C	-4.3362	2.505	0.62119
C	-3.44	1.3628	0.44406
C	-3.8148	3.77578	0.64331
C	-2.412	4.04168	0.51818
C	-1.8891	5.33313	0.54725
H	-4.2307	-4.9989	0.03531
H	-4.6045	-2.5484	0.17187
H	-4.9831	-0.1193	0.35049
H	-4.4819	4.61866	0.80921
H	-2.5692	6.17705	0.64455
H	-0.6449	7.74289	0.58837
H	1.27489	9.31233	0.54837
H	12.1756	5.15268	-0.2398
H	12.5541	2.70566	-0.3913
H	12.9349	0.28131	-0.5192
H	12.4372	-4.4769	-0.8925
H	10.5209	-6.0305	-0.7683
H	8.59587	-7.5949	-0.7284
H	6.67478	-9.1634	-0.7028

H	4.2537	-9.5525	-0.6006
H	1.94291	-8.6635	-0.4465
H	-0.3723	-7.779	-0.2951
H	-2.6879	-6.9007	-0.1415
H	3.69483	9.70317	0.42735
H	6.00503	8.81539	0.2545
H	8.31907	7.93181	0.09072
H	10.6333	7.05497	-0.0652
N	-5.7019	2.26697	0.70572
N	13.6562	-2.1249	-0.831
H	14.1912	-2.9457	-1.0913
H	13.9147	-1.3368	-1.4141
H	-5.9912	1.49865	1.30876
H	-6.2586	3.10316	0.85962
C	-5.4613	-4.763	4.66296
C	-6.1168	-4.8857	3.44155
C	-6.5786	-3.7411	2.7843
C	-6.3603	-2.4514	3.31947
C	-5.6969	-2.3442	4.56184
C	-5.2654	-3.5018	5.22158
H	-5.1116	-5.6481	5.18658
H	-6.2923	-5.8534	2.98557
H	-4.7847	-3.3856	6.18831
C	-8.0036	-2.7508	0.93432
C	-8.8498	-2.9382	-0.1765
C	-9.5764	-1.8457	-0.7125
C	-9.4606	-0.5971	-0.1135
C	-8.5618	-0.3784	0.97167
C	-7.8267	-1.4517	1.49303
C	-6.7895	-1.2479	2.54453
C	-7.3197	-3.9124	1.51226
C	-10.464	-2.1074	-1.9073
C	-10.909	-0.8282	-2.6432
C	-11.374	0.20839	-1.6022
C	-10.247	0.5832	-0.6406
H	-11.356	-2.6635	-1.5893
H	-11.738	1.1144	-2.1016
O	-5.5414	-1.1471	5.19952
O	-7.3883	-5.0389	0.97884
O	-6.2567	-0.157	2.73051
O	-8.4563	0.83049	1.56331

O	-9.0181	-4.1297	-0.7709
H	-8.7306	1.57053	0.98421
H	-8.432	-4.7718	-0.2836
C	-4.2793	-0.4943	5.00496
H	-4.3093	0.40231	5.62682
H	-3.452	-1.1383	5.33073
H	-4.1503	-0.2118	3.95712
O	-13.098	-1.6971	-3.1152
C	-12.093	-1.1609	-3.5572
C	-12.022	-0.7987	-5.0298
H	-11.799	0.27573	-5.1162
H	-11.153	-1.3162	-5.4671
O	-13.213	-1.1286	-5.6891
H	-13.772	-1.5634	-5.0156
O	-9.8747	-0.3085	-3.4725
H	-9.3138	0.27553	-2.9327
O	-9.2608	1.43002	-1.3173
C	-9.437	2.81403	-1.2016
C	-8.3416	3.4997	-2.004
C	-8.3714	5.01723	-1.7722
H	-7.3843	3.08594	-1.6685
C	-9.4353	4.53213	0.4874
C	-8.3601	5.33408	-0.255
O	-9.3172	3.12941	0.1826
O	-7.081	5.04696	0.27721
N	-7.1638	5.62494	-2.3475
C	-9.3741	4.67385	2.0003
H	-10.158	4.0719	2.46873
H	-8.402	4.34683	2.37697
H	-9.5213	5.72073	2.28529
H	-7.2998	6.62021	-2.5154
H	-6.9225	5.19879	-3.2395
H	-6.4689	5.23495	-0.4687
H	-8.4673	3.26934	-3.069
H	-10.446	3.11816	-1.5373
H	-9.303	5.42554	-2.1997
H	-8.5978	6.40464	-0.1175
H	-10.417	4.87742	0.11992
H	-9.9343	-2.7555	-2.6124
H	-10.66	1.15254	0.1985
H	-12.213	-0.2128	-1.0372

E= -5712.6885594 (Hartree)

DOX/O-C2

	X	Y	Z
C	1.91789	-2.6415	0.29645
C	3.21102	-2.6797	-0.203
C	3.62891	-3.5046	-1.29
C	5.85875	-2.4836	-1.308
C	4.90009	-3.4388	-1.7947
C	7.1655	-2.3614	-1.8672
C	2.27935	-0.5807	1.61038
C	1.45575	-1.6162	1.15714
C	3.73281	-0.7124	1.4081
C	4.23236	-1.8338	0.42602
C	6.37968	-0.5892	0.18744
C	5.51943	-1.6204	-0.2496
C	7.67624	-0.4867	-0.3962
C	8.05154	-1.4123	-1.4021
C	2.70384	1.59076	2.65362
C	1.83724	0.5922	2.29927
C	4.09425	1.57348	2.2845
C	4.60249	0.45997	1.58844
C	6.78661	1.5352	1.41536
C	5.92971	0.44093	1.09771
C	8.11795	1.53562	0.88937
C	8.54219	0.56394	0.01513
C	4.97385	2.64589	2.58851
C	6.28977	2.61386	2.19006
H	5.19637	-4.0855	-2.6129
H	9.04532	-1.3393	-1.8416
H	2.90737	-4.1965	-1.7173
H	1.18737	-3.3562	-0.0741
H	0.78548	0.68634	2.54788
H	2.33049	2.4569	3.19388
H	4.59269	3.49628	3.14823
H	6.95921	3.43126	2.43338
H	9.54477	0.61514	-0.4072
O	7.47797	-3.2327	-2.8727

O	8.91281	2.57765	1.27665
O	-0.4643	-2.6128	2.15692
O	-0.7893	-0.6568	1.15977
O	4.31344	-1.9437	1.85175
C	-0.0034	-1.6772	1.53318
H	8.38405	-3.0567	-3.1705
H	9.77778	2.48805	0.84711
H	-0.3709	-0.0619	0.4855
C	0.76311	6.22286	-1.5169
C	-0.505	6.03016	-0.9753
C	-0.9968	4.73258	-0.8077
C	-0.2097	3.60774	-1.141
C	1.0637	3.81856	-1.7109
C	1.53283	5.12487	-1.8968
H	1.14612	7.22884	-1.6635
H	-1.1352	6.86508	-0.6903
H	2.5043	5.25771	-2.3636
C	-2.9758	3.2202	-0.3495
C	-4.3427	3.06627	-0.053
C	-4.966	1.79932	-0.1926
C	-4.2218	0.72467	-0.6626
C	-2.8215	0.84877	-0.9052
C	-2.195	2.08799	-0.7243
C	-0.7225	2.24372	-0.8226
C	-2.3793	4.55731	-0.2975
C	-6.4325	1.69465	0.15539
C	-6.93	0.24386	0.30865
C	-6.4012	-0.5877	-0.8766
C	-4.8726	-0.6209	-0.8965
H	-7.0333	2.19892	-0.6124
H	-6.7819	-1.6148	-0.8252
O	1.80741	2.77893	-2.1883
O	-3.0262	5.54675	0.09987
O	0.06421	1.32466	-0.5798
O	-2.0928	-0.1738	-1.3948
O	-5.1167	4.08353	0.35616
H	-2.4502	-1.0578	-1.1634
H	-4.5277	4.88621	0.39464
C	2.89261	2.34658	-1.357
H	3.4075	1.56582	-1.9195
H	3.58917	3.17072	-1.155

H	2.51244	1.93768	-0.4181
O	-9.0728	0.753	-0.6534
C	-8.4615	0.22831	0.26456
C	-9.2282	-0.4742	1.37109
H	-8.8611	-1.509	1.45056
H	-8.9656	0.00608	2.32711
O	-10.608	-0.4378	1.12932
H	-10.714	0.08601	0.31138
O	-6.5404	-0.3172	1.55757
H	-5.671	-0.7424	1.44792
O	-4.3694	-1.4917	0.16403
C	-4.1239	-2.8253	-0.2
C	-3.6347	-3.5812	1.0246
C	-3.1827	-4.9962	0.63172
H	-2.7956	-3.0298	1.46242
C	-2.7267	-4.0903	-1.6952
C	-2.1758	-4.9443	-0.5449
O	-3.125	-2.7917	-1.2125
O	-0.94	-4.4219	-0.1169
N	-2.4992	-5.6205	1.76804
C	-1.7303	-3.8615	-2.8203
H	-2.1776	-3.246	-3.6067
H	-0.8399	-3.3585	-2.436
H	-1.4291	-4.82	-3.2561
H	-2.4794	-6.6339	1.67364
H	-2.962	-5.4017	2.64676
H	-0.8956	-4.5838	0.8491
H	-4.4421	-3.6324	1.76613
H	-5.0317	-3.2885	-0.6303
H	-4.0644	-5.5677	0.28923
H	-2.0477	-5.972	-0.9356
H	-3.6264	-4.595	-2.0876
H	-6.6168	2.23263	1.09093
H	-4.5294	-1.0247	-1.8543
H	-6.7728	-0.1472	-1.8082

E= -3264.5809872 (Hartree)

DOX/O-A-C2

	X	Y	Z
C	-3.6138	0.69919	-1.4039
C	-2.2782	0.75373	-1.7657
C	-1.6441	-0.177	-2.6379
C	0.46558	1.09694	-2.6013
C	-0.3323	-0.0292	-3.006
C	1.83549	1.26013	-3.0096
C	-3.6645	2.9833	-0.4546
C	-4.2977	1.77919	-0.789
C	-2.1879	3.02054	-0.5157
C	-1.4473	1.83238	-1.2148
C	0.5527	3.29193	-1.4735
C	-0.1137	2.08984	-1.7844
C	1.89412	3.46272	-1.9323
C	2.51362	2.4189	-2.6553
C	-3.6076	5.33306	0.22842
C	-4.3064	4.17724	0.00191
C	-2.2004	5.45172	-0.0371
C	-1.4899	4.31661	-0.4733
C	0.55353	5.63963	-0.6517
C	-0.1237	4.39691	-0.8309
C	1.93053	5.73182	-1.0405
C	2.57154	4.68447	-1.6578
C	-1.5011	6.67513	0.13195
C	-0.1556	6.75774	-0.1448
H	0.0976	-0.761	-3.6819
H	3.54848	2.54218	-2.966
H	-2.2179	-1.0219	-3.006
H	-4.2019	-0.1621	-1.7073
H	-5.3733	4.16983	0.19763
H	-4.1356	6.21107	0.5898
H	-2.0423	7.54816	0.48596
H	0.37381	7.69383	-0.007
H	3.60482	4.79638	-1.979
O	2.53828	6.92613	-0.7902
O	-6.2276	0.56161	-0.07
O	-6.618	2.50355	-1.0526
O	-1.5236	1.97284	0.21549

C	-5.767	1.55858	-0.5942
H	3.45296	6.89747	-1.1165
H	-6.1357	3.17719	-1.5645
N	2.44975	0.29175	-3.7996
H	3.45846	0.38317	-3.8492
H	2.19934	-0.6704	-3.5991
C	7.66546	0.01826	0.48973
C	6.74223	-0.5037	-0.4114
C	5.44079	-0.7926	0.01338
C	5.02626	-0.5352	1.33962
C	5.98264	-0.0238	2.24487
C	7.28748	0.24328	1.81199
H	8.68028	0.23499	0.17059
H	7.0142	-0.7083	-1.4403
H	8.00127	0.61728	2.53965
C	3.21687	-1.9088	-0.476
C	2.40872	-2.652	-1.3567
C	1.19373	-3.2247	-0.9118
C	0.79109	-3.0117	0.4004
C	1.55097	-2.184	1.282
C	2.78294	-1.6564	0.85929
C	3.60311	-0.7774	1.74252
C	4.51021	-1.4124	-0.9541
C	0.42393	-4.0867	-1.8869
C	-1.0078	-4.4392	-1.4389
C	-0.9987	-4.7941	0.0616
C	-0.4958	-3.6256	0.90765
H	0.98268	-5.0167	-2.052
H	-2.0041	-5.0723	0.39579
O	5.70813	0.14233	3.57684
O	4.85729	-1.5479	-2.1489
O	3.13993	-0.2421	2.74508
O	1.1414	-1.9684	2.54847
O	2.74718	-2.8615	-2.6475
H	0.17037	-2.0751	2.66713
H	3.64827	-2.4425	-2.7633
C	5.36059	1.47723	3.97276
H	5.25252	1.45174	5.05875
H	6.15309	2.18516	3.7014
H	4.41388	1.77576	3.5144
O	-0.817	-6.6763	-2.3104

C	-1.4965	-5.6643	-2.2177
C	-2.8706	-5.6291	-2.8637
H	-3.616	-5.3723	-2.0972
H	-2.885	-4.8037	-3.5914
O	-3.1676	-6.8617	-3.4751
H	-2.3701	-7.411	-3.3391
O	-1.9189	-3.3775	-1.7155
H	-1.9579	-2.8001	-0.9296
O	-1.4793	-2.5417	0.90566
C	-2.3559	-2.5067	2.00533
C	-3.4062	-1.4381	1.75907
C	-4.2775	-1.2408	3.00879
H	-2.8905	-0.5034	1.51357
C	-2.2977	-2.0825	4.37457
C	-3.3907	-1.0147	4.26005
O	-1.5567	-2.1749	3.13782
O	-2.8104	0.27711	4.19109
N	-5.1042	-0.0369	2.83769
C	-1.2886	-1.8164	5.48023
H	-0.5354	-2.6098	5.50536
H	-0.7918	-0.8564	5.31788
H	-1.7948	-1.7883	6.45051
H	-5.9091	-0.0728	3.46153
H	-5.4671	0.02418	1.88562
H	-3.5023	0.79649	3.72218
H	-4.0271	-1.7211	0.90219
H	-2.8096	-3.4966	2.17607
H	-4.876	-2.1509	3.17159
H	-4.0265	-1.105	5.15875
H	-2.7929	-3.051	4.54591
H	0.37125	-3.5837	-2.8575
H	-0.361	-3.9654	1.93886
H	-0.3467	-5.6595	0.21949

E= -3244.7120297 (Hartree)