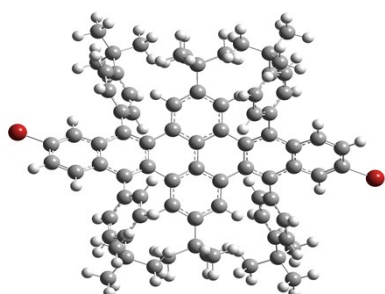
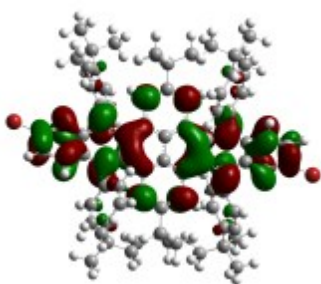


Optimized structures, Z-matrices (in Å) of the ground states and their corresponding total SCF (ESCF) and zero-point (EZP) energies (in Hartree). There are no imaginary frequencies for the intermediates **3**.

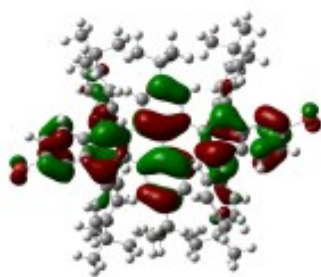
**3i**



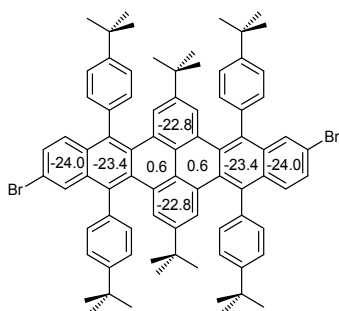
Optimized structure



LUMO = -1.66 eV

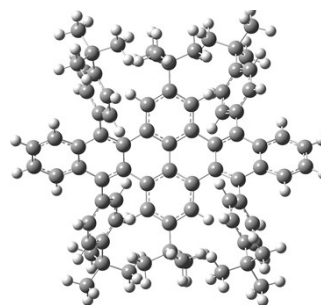


HOMO = -5.19 eV

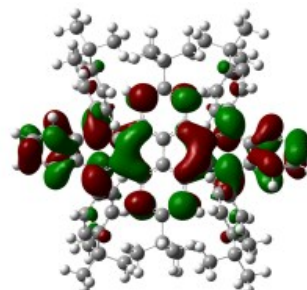


NICS(1)zz

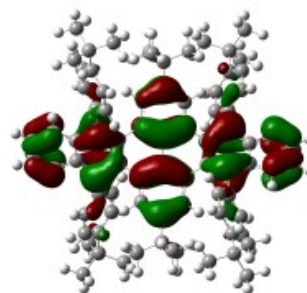
**3a**



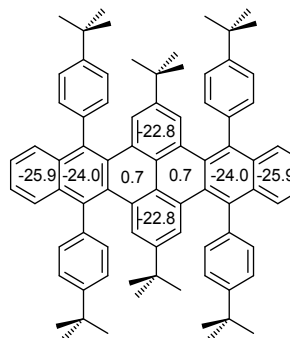
Optimized structure



LUMO = -1.42 eV



HOMO = -5.00 eV



NICS(1)zz

C	5.0327	5.0898	10.5352	C	3.8275	4.7133	11.0781
H	5.06405	5.9083	10.04875	C	5.0327	5.0898	10.5352
C	6.262	4.5539	11.034	H	5.0501	5.7014	9.8349
C	6.2043	3.6924	12.1764	C	6.262	4.5539	11.034
C	4.9378	3.2485	12.6422	C	6.2043	3.6924	12.1764
H	4.8927	2.6074	13.3157	C	4.9378	3.2485	12.6422
C	7.4282	3.3899	12.8594	H	4.8927	2.6074	13.3157
C	8.6435	3.87	12.3495	C	7.4282	3.3899	12.8594
C	8.6879	4.3944	11.0136	C	8.6435	3.87	12.3495
C	7.5106	4.8498	10.4203	C	8.6879	4.3944	11.0136
C	7.5133	5.7589	9.2386	C	7.5106	4.8498	10.4203
C	6.8853	5.4499	8.0426	C	7.5133	5.7589	9.2386
H	6.4584	4.6295	7.9466	C	6.8853	5.4499	8.0426
C	6.8845	6.3508	6.9773	H	6.4584	4.6295	7.9466
H	6.4534	6.1206	6.1874	C	6.8845	6.3508	6.9773
C	7.5162	7.5871	7.0749	H	6.4534	6.1206	6.1874
C	8.1416	7.8961	8.2897	C	7.5162	7.5871	7.0749
H	8.5613	8.7214	8.3872	C	8.1416	7.8961	8.2897
C	8.1488	7.0002	9.3519	H	8.5613	8.7214	8.3872
H	8.5823	7.2287	10.1434	C	8.1488	7.0002	9.3519
C	6.5889	9.7818	6.3683	H	8.5823	7.2287	10.1434
H	6.5511	10.4312	5.6618	C	6.5889	9.7818	6.3683
H	6.9474	10.1928	7.1598	H	6.5511	10.4312	5.6618
H	5.7055	9.4546	6.5493	H	6.9474	10.1928	7.1598
C	7.488	8.6195	5.9466	H	5.7055	9.4546	6.5493
C	6.946	8.054	4.6421	C	7.488	8.6195	5.9466
H	6.83	8.7642	4.0079	C	6.946	8.054	4.6421
H	6.1017	7.6282	4.8042	H	6.83	8.7642	4.0079
H	7.5655	7.4095	4.2912	H	6.1017	7.6282	4.8042
C	8.9036	9.1456	5.6665	H	7.5655	7.4095	4.2912
H	9.4739	8.414	5.4179	C	8.9036	9.1456	5.6665
H	9.252	9.5648	6.4564	H	9.4739	8.414	5.4179
H	8.8747	9.7851	4.9521	H	9.252	9.5648	6.4564
C	7.3848	2.5498	14.0852	H	8.8747	9.7851	4.9521
C	8.1839	1.4089	14.1906	C	7.3848	2.5498	14.0852
H	8.7242	1.1623	13.4747	C	8.1839	1.4089	14.1906

C	8.1883	0.6412	15.3394	H	8.7242	1.1623	13.4747
H	8.7388	-0.1085	15.3756	C	8.1883	0.6412	15.3394
C	7.4004	0.9502	16.444	H	8.7388	-0.1085	15.3756
C	6.6152	2.0945	16.3528	C	7.4004	0.9502	16.444
H	6.089	2.3443	17.0782	C	6.6152	2.0945	16.3528
C	6.6004	2.8737	15.204	H	6.089	2.3443	17.0782
H	6.0593	3.63	15.1741	C	6.6004	2.8737	15.204
C	7.3605	0.0543	17.6809	H	6.0593	3.63	15.1741
C	8.7078	-0.5458	17.9704	C	7.3605	0.0543	17.6809
H	9.2686	0.1151	18.3827	C	8.7078	-0.5458	17.9704
H	9.1087	-0.8401	17.1506	H	9.2686	0.1151	18.3827
H	8.6025	-1.2938	18.5637	H	9.1087	-0.8401	17.1506
C	6.4419	-1.1656	17.3599	H	8.6025	-1.2938	18.5637
H	6.4456	-1.7739	18.1042	C	6.4419	-1.1656	17.3599
H	6.7696	-1.6161	16.5794	H	6.4456	-1.7739	18.1042
H	5.548	-0.8598	17.2009	H	6.7696	-1.6161	16.5794
C	6.6074	0.7151	18.8453	H	5.548	-0.8598	17.2009
H	7.1687	1.3777	19.2545	C	6.6074	0.7151	18.8453
H	6.3745	0.0477	19.4952	H	7.1687	1.3777	19.2545
H	5.8093	1.1311	18.5149	H	6.3745	0.0477	19.4952
C	10.0028	4.3517	10.3243	H	5.8093	1.1311	18.5149
C	11.1759	4.1462	11.0797	C	10.0028	4.3517	10.3243
C	12.4265	3.9883	10.4392	C	11.1759	4.1462	11.0797
C	12.4732	4.1264	9.0497	C	12.4265	3.9883	10.4392
H	13.2989	4.087	8.6249	C	12.4732	4.1264	9.0497
C	11.3343	4.3204	8.2787	H	13.2989	4.087	8.6249
C	10.111	4.3845	8.9286	C	11.3343	4.3204	8.2787
H	9.3346	4.452	8.4203	C	10.111	4.3845	8.9286
C	11.432	4.4158	6.746	H	9.3346	4.452	8.4203
C	11.2171	3.0135	6.2015	C	11.432	4.4158	6.746
H	12.0675	2.5942	6.0505	C	11.2171	3.0135	6.2015
H	10.735	3.0611	5.3722	H	12.0675	2.5942	6.0505
H	10.715	2.4956	6.8357	H	10.735	3.0611	5.3722
C	12.7193	4.863	6.2881	H	10.715	2.4956	6.8357
H	12.8102	5.8033	6.4564	C	12.7193	4.863	6.2881
H	12.7974	4.6969	5.3455	H	12.8102	5.8033	6.4564

H	13.4088	4.3845	6.7554	H	12.7974	4.6969	5.3455
C	10.3702	5.2937	6.159	H	13.4088	4.3845	6.7554
H	10.3871	6.1502	6.5933	C	10.3702	5.2937	6.159
H	9.5102	4.886	6.2881	H	10.3871	6.1502	6.5933
H	10.5306	5.4071	5.2196	H	9.5102	4.886	6.2881
C	17.2512	5.0898	13.0687	H	10.5306	5.4071	5.2196
H	17.21997	5.9083	13.55506	C	18.4565	4.7133	12.5258
C	16.0219	4.5539	12.5698	C	17.2512	5.0898	13.0687
C	16.0796	3.6924	11.4274	C	16.0219	4.5539	12.5698
C	17.3462	3.2485	10.9616	C	16.0796	3.6924	11.4274
H	17.3913	2.6074	10.2881	C	17.3462	3.2485	10.9616
C	14.8557	3.3899	10.7445	H	17.3913	2.6074	10.2881
C	13.6404	3.87	11.2543	C	14.8557	3.3899	10.7445
C	13.5961	4.3944	12.5903	C	13.6404	3.87	11.2543
C	14.7733	4.8498	13.1835	C	13.5961	4.3944	12.5903
C	14.7707	5.7589	14.3653	C	14.7733	4.8498	13.1835
C	15.3987	5.4499	15.5612	C	14.7707	5.7589	14.3653
H	15.8256	4.6295	15.6572	C	15.3987	5.4499	15.5612
C	15.3994	6.3508	16.6266	H	15.8256	4.6295	15.6572
H	15.8306	6.1206	17.4165	C	15.3994	6.3508	16.6266
C	14.7677	7.5871	16.529	H	15.8306	6.1206	17.4165
C	14.1424	7.8961	15.3142	C	14.7677	7.5871	16.529
H	13.7227	8.7214	15.2166	C	14.1424	7.8961	15.3142
C	14.1352	7.0002	14.252	H	13.7227	8.7214	15.2166
H	13.7017	7.2287	13.4605	C	14.1352	7.0002	14.252
C	15.6951	9.7818	17.2355	H	13.7017	7.2287	13.4605
H	15.7329	10.4312	17.9421	C	15.6951	9.7818	17.2355
H	15.3366	10.1928	16.444	H	15.7329	10.4312	17.9421
H	16.5784	9.4546	17.0546	H	15.3366	10.1928	16.444
C	14.796	8.6195	17.6573	H	16.5784	9.4546	17.0546
C	15.3379	8.054	18.9618	C	14.796	8.6195	17.6573
H	15.4539	8.7642	19.5959	C	15.3379	8.054	18.9618
H	16.1822	7.6282	18.7997	H	15.4539	8.7642	19.5959
H	14.7185	7.4095	19.3127	H	16.1822	7.6282	18.7997
C	13.3804	9.1456	17.9374	H	14.7185	7.4095	19.3127
H	12.8101	8.414	18.186	C	13.3804	9.1456	17.9374

H	13.032	9.5648	17.1474	H	12.8101	8.414	18.186
H	13.4093	9.7851	18.6518	H	13.032	9.5648	17.1474
C	14.8992	2.5498	9.5187	H	13.4093	9.7851	18.6518
C	14.1001	1.4089	9.4132	C	14.8992	2.5498	9.5187
H	13.5598	1.1623	10.1292	C	14.1001	1.4089	9.4132
C	14.0956	0.6412	8.2645	H	13.5598	1.1623	10.1292
H	13.5451	-0.1085	8.2283	C	14.0956	0.6412	8.2645
C	14.8836	0.9502	7.1598	H	13.5451	-0.1085	8.2283
C	15.6688	2.0945	7.2511	C	14.8836	0.9502	7.1598
H	16.195	2.3443	6.5257	C	15.6688	2.0945	7.2511
C	15.6836	2.8737	8.3998	H	16.195	2.3443	6.5257
H	16.2247	3.63	8.4297	C	15.6836	2.8737	8.3998
C	14.9235	0.0543	5.923	H	16.2247	3.63	8.4297
C	13.5761	-0.5458	5.6335	C	14.9235	0.0543	5.923
H	13.0154	0.1151	5.2212	C	13.5761	-0.5458	5.6335
H	13.1753	-0.8401	6.4533	H	13.0154	0.1151	5.2212
H	13.6815	-1.2938	5.0402	H	13.1753	-0.8401	6.4533
C	15.842	-1.1656	6.244	H	13.6815	-1.2938	5.0402
H	15.8384	-1.7739	5.4997	C	15.842	-1.1656	6.244
H	15.5143	-1.6161	7.0245	H	15.8384	-1.7739	5.4997
H	16.736	-0.8598	6.4029	H	15.5143	-1.6161	7.0245
C	15.6766	0.7151	4.7585	H	16.736	-0.8598	6.4029
H	15.1153	1.3777	4.3494	C	15.6766	0.7151	4.7585
H	15.9095	0.0477	4.1086	H	15.1153	1.3777	4.3494
H	16.4747	1.1311	5.089	H	15.9095	0.0477	4.1086
C	12.2812	4.3517	13.2795	H	16.4747	1.1311	5.089
C	11.1081	4.1462	12.5242	C	12.2812	4.3517	13.2795
C	9.8575	3.9883	13.1647	C	11.1081	4.1462	12.5242
C	9.8107	4.1264	14.5541	C	9.8575	3.9883	13.1647
H	8.9851	4.087	14.979	C	9.8107	4.1264	14.5541
C	10.9497	4.3204	15.3252	H	8.9851	4.087	14.979
C	12.173	4.3845	14.6753	C	10.9497	4.3204	15.3252
H	12.9493	4.452	15.1836	C	12.173	4.3845	14.6753
C	10.852	4.4158	16.8579	H	12.9493	4.452	15.1836
C	11.0669	3.0135	17.4023	C	10.852	4.4158	16.8579
H	10.2165	2.5942	17.5534	C	11.0669	3.0135	17.4023

H	11.549	3.0611	18.2316	H	10.2165	2.5942	17.5534
H	11.5689	2.4956	16.7682	H	11.549	3.0611	18.2316
C	9.5647	4.863	17.3158	H	11.5689	2.4956	16.7682
H	9.4738	5.8033	17.1474	C	9.5647	4.863	17.3158
H	9.4865	4.6969	18.2584	H	9.4738	5.8033	17.1474
H	8.8752	4.3845	16.8484	H	9.4865	4.6969	18.2584
C	11.9138	5.2937	17.4448	H	8.8752	4.3845	16.8484
H	11.8968	6.1502	17.0105	C	11.9138	5.2937	17.4448
H	12.7738	4.886	17.3158	H	11.8968	6.1502	17.0105
H	11.7534	5.4071	18.3843	H	12.7738	4.886	17.3158
C	3.7752	3.7582	12.1056	H	11.7534	5.4071	18.3843
H	3.25201	2.88112	11.41781	C	3.7752	3.7582	12.1056
C	18.5087	3.7582	11.4982	C	18.5087	3.7582	11.4982
H	19.03108	2.87984	12.18502	H	17.23129	5.79358	13.87443
Br	2.6227	5.31795	10.57168	H	19.4561	3.42424	11.12968
Br	19.66133	5.31786	13.03225	H	19.36234	5.15171	12.88932
C	3.8275	4.7133	11.0781	H	2.92167	5.15177	10.71461
C	18.4565	4.7133	12.5258	H	2.82779	3.42421	12.47407

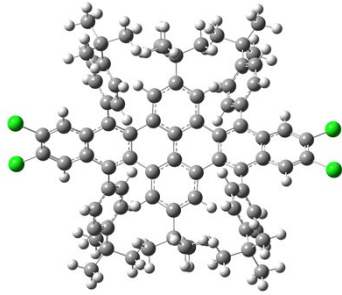
E(SCF)=-8240.35804999 a.u.

E(zp)=-8238.985576 a.u.

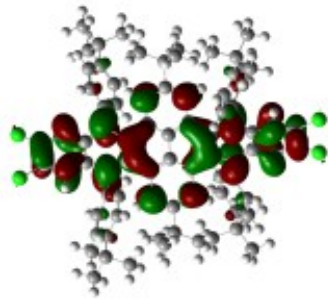
E(SCF) = -3098.14922207 a.u.

E(zp)=-3096.757062 a.u.

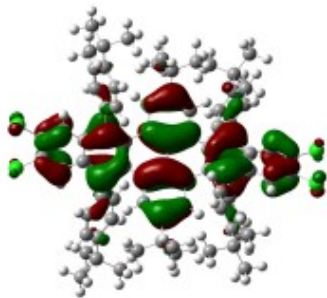
**3d**



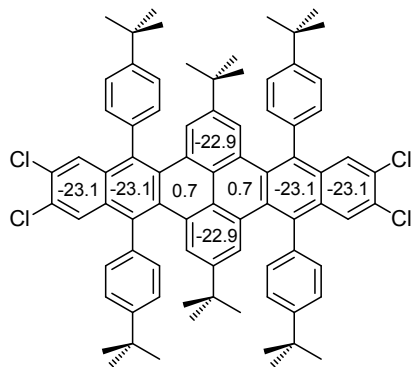
Optimized structure



LUMO = -1.83 eV

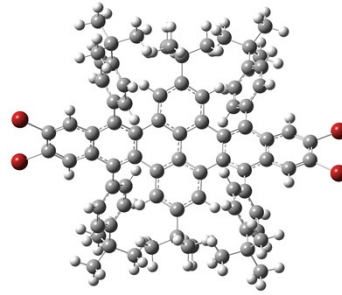


HOMO = -5.34 eV

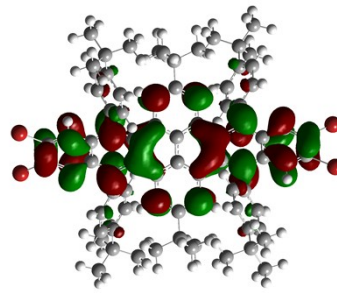


NICS(1)zz

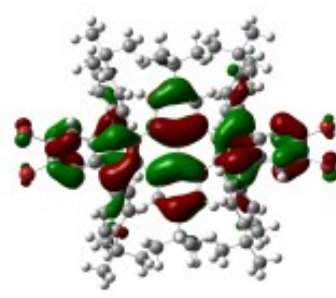
**3e**



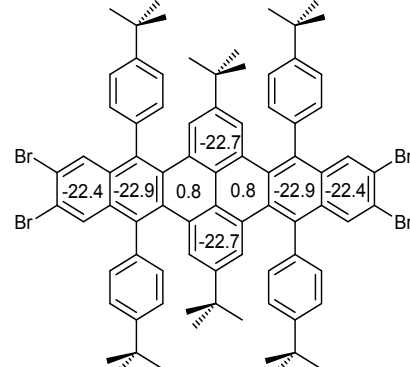
Optimized structure



LUMO = -1.83 eV



HOMO = -5.32 eV



NICS(1)zz

C	3.8275	4.7133	11.0781	C	3.8275	4.7133	11.0781
C	5.0327	5.0898	10.5352	C	5.0327	5.0898	10.5352
H	5.0501	5.7014	9.8349	H	5.0501	5.7014	9.8349
C	6.262	4.5539	11.034	C	6.262	4.5539	11.034
C	6.2043	3.6924	12.1764	C	6.2043	3.6924	12.1764
C	4.9378	3.2485	12.6422	C	4.9378	3.2485	12.6422
H	4.8927	2.6074	13.3157	H	4.8927	2.6074	13.3157
C	7.4282	3.3899	12.8594	C	7.4282	3.3899	12.8594
C	8.6435	3.87	12.3495	C	8.6435	3.87	12.3495
C	8.6879	4.3944	11.0136	C	8.6879	4.3944	11.0136
C	7.5106	4.8498	10.4203	C	7.5106	4.8498	10.4203
C	7.5133	5.7589	9.2386	C	7.5133	5.7589	9.2386
C	6.8853	5.4499	8.0426	C	6.8853	5.4499	8.0426
H	6.4584	4.6295	7.9466	H	6.4584	4.6295	7.9466
C	6.8845	6.3508	6.9773	C	6.8845	6.3508	6.9773
H	6.4534	6.1206	6.1874	H	6.4534	6.1206	6.1874
C	7.5162	7.5871	7.0749	C	7.5162	7.5871	7.0749
C	8.1416	7.8961	8.2897	C	8.1416	7.8961	8.2897
H	8.5613	8.7214	8.3872	H	8.5613	8.7214	8.3872
C	8.1488	7.0002	9.3519	C	8.1488	7.0002	9.3519
H	8.5823	7.2287	10.1434	H	8.5823	7.2287	10.1434
C	6.5889	9.7818	6.3683	C	6.5889	9.7818	6.3683
H	6.5511	10.4312	5.6618	H	6.5511	10.4312	5.6618
H	6.9474	10.1928	7.1598	H	6.9474	10.1928	7.1598
H	5.7055	9.4546	6.5493	H	5.7055	9.4546	6.5493
C	7.488	8.6195	5.9466	C	7.488	8.6195	5.9466
C	6.946	8.054	4.6421	C	6.946	8.054	4.6421
H	6.83	8.7642	4.0079	H	6.83	8.7642	4.0079
H	6.1017	7.6282	4.8042	H	6.1017	7.6282	4.8042
H	7.5655	7.4095	4.2912	H	7.5655	7.4095	4.2912
C	8.9036	9.1456	5.6665	C	8.9036	9.1456	5.6665
H	9.4739	8.414	5.4179	H	9.4739	8.414	5.4179
H	9.252	9.5648	6.4564	H	9.252	9.5648	6.4564
H	8.8747	9.7851	4.9521	H	8.8747	9.7851	4.9521
C	7.3848	2.5498	14.0852	C	7.3848	2.5498	14.0852
C	8.1839	1.4089	14.1906	C	8.1839	1.4089	14.1906



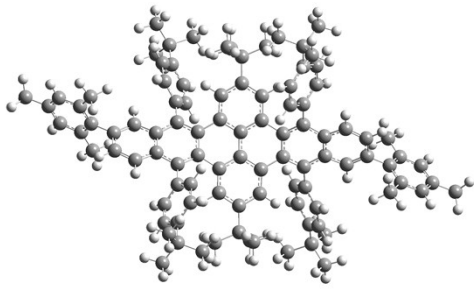
H	8.7242	1.1623	13.4747	H	8.7242	1.1623	13.4747
C	8.1883	0.6412	15.3394	C	8.1883	0.6412	15.3394
H	8.7388	-0.1085	15.3756	H	8.7388	-0.1085	15.3756
C	7.4004	0.9502	16.444	C	7.4004	0.9502	16.444
C	6.6152	2.0945	16.3528	C	6.6152	2.0945	16.3528
H	6.089	2.3443	17.0782	H	6.089	2.3443	17.0782
C	6.6004	2.8737	15.204	C	6.6004	2.8737	15.204
H	6.0593	3.63	15.1741	H	6.0593	3.63	15.1741
C	7.3605	0.0543	17.6809	C	7.3605	0.0543	17.6809
C	8.7078	-0.5458	17.9704	C	8.7078	-0.5458	17.9704
H	9.2686	0.1151	18.3827	H	9.2686	0.1151	18.3827
H	9.1087	-0.8401	17.1506	H	9.1087	-0.8401	17.1506
H	8.6025	-1.2938	18.5637	H	8.6025	-1.2938	18.5637
C	6.4419	-1.1656	17.3599	C	6.4419	-1.1656	17.3599
H	6.4456	-1.7739	18.1042	H	6.4456	-1.7739	18.1042
H	6.7696	-1.6161	16.5794	H	6.7696	-1.6161	16.5794
H	5.548	-0.8598	17.2009	H	5.548	-0.8598	17.2009
C	6.6074	0.7151	18.8453	C	6.6074	0.7151	18.8453
H	7.1687	1.3777	19.2545	H	7.1687	1.3777	19.2545
H	6.3745	0.0477	19.4952	H	6.3745	0.0477	19.4952
H	5.8093	1.1311	18.5149	H	5.8093	1.1311	18.5149
C	10.0028	4.3517	10.3243	C	10.0028	4.3517	10.3243
C	11.1759	4.1462	11.0797	C	11.1759	4.1462	11.0797
C	12.4265	3.9883	10.4392	C	12.4265	3.9883	10.4392
C	12.4732	4.1264	9.0497	C	12.4732	4.1264	9.0497
H	13.2989	4.087	8.6249	H	13.2989	4.087	8.6249
C	11.3343	4.3204	8.2787	C	11.3343	4.3204	8.2787
C	10.111	4.3845	8.9286	C	10.111	4.3845	8.9286
H	9.3346	4.452	8.4203	H	9.3346	4.452	8.4203
C	11.432	4.4158	6.746	C	11.432	4.4158	6.746
C	11.2171	3.0135	6.2015	C	11.2171	3.0135	6.2015
H	12.0675	2.5942	6.0505	H	12.0675	2.5942	6.0505
H	10.735	3.0611	5.3722	H	10.735	3.0611	5.3722
H	10.715	2.4956	6.8357	H	10.715	2.4956	6.8357
C	12.7193	4.863	6.2881	C	12.7193	4.863	6.2881
H	12.8102	5.8033	6.4564	H	12.8102	5.8033	6.4564

H	12.7974	4.6969	5.3455	H	12.7974	4.6969	5.3455
H	13.4088	4.3845	6.7554	H	13.4088	4.3845	6.7554
C	10.3702	5.2937	6.159	C	10.3702	5.2937	6.159
H	10.3871	6.1502	6.5933	H	10.3871	6.1502	6.5933
H	9.5102	4.886	6.2881	H	9.5102	4.886	6.2881
H	10.5306	5.4071	5.2196	H	10.5306	5.4071	5.2196
C	18.4565	4.7133	12.5258	C	18.4565	4.7133	12.5258
C	17.2512	5.0898	13.0687	C	17.2512	5.0898	13.0687
C	16.0219	4.5539	12.5698	C	16.0219	4.5539	12.5698
C	16.0796	3.6924	11.4274	C	16.0796	3.6924	11.4274
C	17.3462	3.2485	10.9616	C	17.3462	3.2485	10.9616
H	17.3913	2.6074	10.2881	H	17.3913	2.6074	10.2881
C	14.8557	3.3899	10.7445	C	14.8557	3.3899	10.7445
C	13.6404	3.87	11.2543	C	13.6404	3.87	11.2543
C	13.5961	4.3944	12.5903	C	13.5961	4.3944	12.5903
C	14.7733	4.8498	13.1835	C	14.7733	4.8498	13.1835
C	14.7707	5.7589	14.3653	C	14.7707	5.7589	14.3653
C	15.3987	5.4499	15.5612	C	15.3987	5.4499	15.5612
H	15.8256	4.6295	15.6572	H	15.8256	4.6295	15.6572
C	15.3994	6.3508	16.6266	C	15.3994	6.3508	16.6266
H	15.8306	6.1206	17.4165	H	15.8306	6.1206	17.4165
C	14.7677	7.5871	16.529	C	14.7677	7.5871	16.529
C	14.1424	7.8961	15.3142	C	14.1424	7.8961	15.3142
H	13.7227	8.7214	15.2166	H	13.7227	8.7214	15.2166
C	14.1352	7.0002	14.252	C	14.1352	7.0002	14.252
H	13.7017	7.2287	13.4605	H	13.7017	7.2287	13.4605
C	15.6951	9.7818	17.2355	C	15.6951	9.7818	17.2355
H	15.7329	10.4312	17.9421	H	15.7329	10.4312	17.9421
H	15.3366	10.1928	16.444	H	15.3366	10.1928	16.444
H	16.5784	9.4546	17.0546	H	16.5784	9.4546	17.0546
C	14.796	8.6195	17.6573	C	14.796	8.6195	17.6573
C	15.3379	8.054	18.9618	C	15.3379	8.054	18.9618
H	15.4539	8.7642	19.5959	H	15.4539	8.7642	19.5959
H	16.1822	7.6282	18.7997	H	16.1822	7.6282	18.7997
H	14.7185	7.4095	19.3127	H	14.7185	7.4095	19.3127
C	13.3804	9.1456	17.9374	C	13.3804	9.1456	17.9374

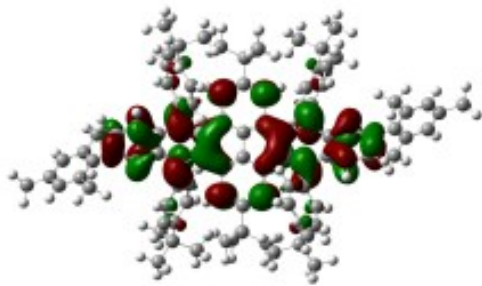
H	12.8101	8.414	18.186	H	12.8101	8.414	18.186
H	13.032	9.5648	17.1474	H	13.032	9.5648	17.1474
H	13.4093	9.7851	18.6518	H	13.4093	9.7851	18.6518
C	14.8992	2.5498	9.5187	C	14.8992	2.5498	9.5187
C	14.1001	1.4089	9.4132	C	14.1001	1.4089	9.4132
H	13.5598	1.1623	10.1292	H	13.5598	1.1623	10.1292
C	14.0956	0.6412	8.2645	C	14.0956	0.6412	8.2645
H	13.5451	-0.1085	8.2283	H	13.5451	-0.1085	8.2283
C	14.8836	0.9502	7.1598	C	14.8836	0.9502	7.1598
C	15.6688	2.0945	7.2511	C	15.6688	2.0945	7.2511
H	16.195	2.3443	6.5257	H	16.195	2.3443	6.5257
C	15.6836	2.8737	8.3998	C	15.6836	2.8737	8.3998
H	16.2247	3.63	8.4297	H	16.2247	3.63	8.4297
C	14.9235	0.0543	5.923	C	14.9235	0.0543	5.923
C	13.5761	-0.5458	5.6335	C	13.5761	-0.5458	5.6335
H	13.0154	0.1151	5.2212	H	13.0154	0.1151	5.2212
H	13.1753	-0.8401	6.4533	H	13.1753	-0.8401	6.4533
H	13.6815	-1.2938	5.0402	H	13.6815	-1.2938	5.0402
C	15.842	-1.1656	6.244	C	15.842	-1.1656	6.244
H	15.8384	-1.7739	5.4997	H	15.8384	-1.7739	5.4997
H	15.5143	-1.6161	7.0245	H	15.5143	-1.6161	7.0245
H	16.736	-0.8598	6.4029	H	16.736	-0.8598	6.4029
C	15.6766	0.7151	4.7585	C	15.6766	0.7151	4.7585
H	15.1153	1.3777	4.3494	H	15.1153	1.3777	4.3494
H	15.9095	0.0477	4.1086	H	15.9095	0.0477	4.1086
H	16.4747	1.1311	5.089	H	16.4747	1.1311	5.089
C	12.2812	4.3517	13.2795	C	12.2812	4.3517	13.2795
C	11.1081	4.1462	12.5242	C	11.1081	4.1462	12.5242
C	9.8575	3.9883	13.1647	C	9.8575	3.9883	13.1647
C	9.8107	4.1264	14.5541	C	9.8107	4.1264	14.5541
H	8.9851	4.087	14.979	H	8.9851	4.087	14.979
C	10.9497	4.3204	15.3252	C	10.9497	4.3204	15.3252
C	12.173	4.3845	14.6753	C	12.173	4.3845	14.6753
H	12.9493	4.452	15.1836	H	12.9493	4.452	15.1836
C	10.852	4.4158	16.8579	C	10.852	4.4158	16.8579
C	11.0669	3.0135	17.4023	C	11.0669	3.0135	17.4023

H	10.2165	2.5942	17.5534	H	10.2165	2.5942	17.5534
H	11.549	3.0611	18.2316	H	11.549	3.0611	18.2316
H	11.5689	2.4956	16.7682	H	11.5689	2.4956	16.7682
C	9.5647	4.863	17.3158	C	9.5647	4.863	17.3158
H	9.4738	5.8033	17.1474	H	9.4738	5.8033	17.1474
H	9.4865	4.6969	18.2584	H	9.4865	4.6969	18.2584
H	8.8752	4.3845	16.8484	H	8.8752	4.3845	16.8484
C	11.9138	5.2937	17.4448	C	11.9138	5.2937	17.4448
H	11.8968	6.1502	17.0105	H	11.8968	6.1502	17.0105
H	12.7738	4.886	17.3158	H	12.7738	4.886	17.3158
H	11.7534	5.4071	18.3843	H	11.7534	5.4071	18.3843
C	3.7752	3.7582	12.1056	C	3.7752	3.7582	12.1056
C	18.5087	3.7582	11.4982	C	18.5087	3.7582	11.4982
Cl	20.00467	5.47921	12.86366	H	17.23129	5.79358	13.87443
Cl	2.80864	2.46499	11.4049	Br	2.72627	2.35478	11.34518
Cl	2.27933	5.47921	10.74024	Br	2.14738	5.54449	10.71145
Cl	19.47393	2.46305	12.19714	Br	19.5562	2.35267	12.25671
H	17.23129	5.79358	13.87443	Br	20.13662	5.54449	12.89245
E(SCF)=-4936.51891882 a.u.				E(SCF)=-13382.55816870 a.u.			
E(zp)=-4935.16615 a.u.				E(zp)=-13381.206437 a.u.			

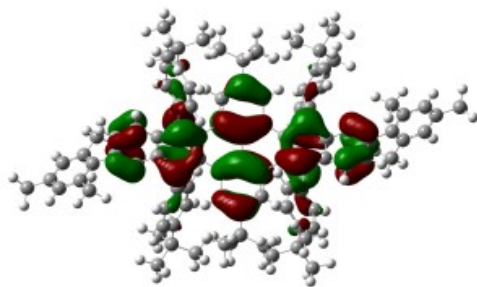
**3k**



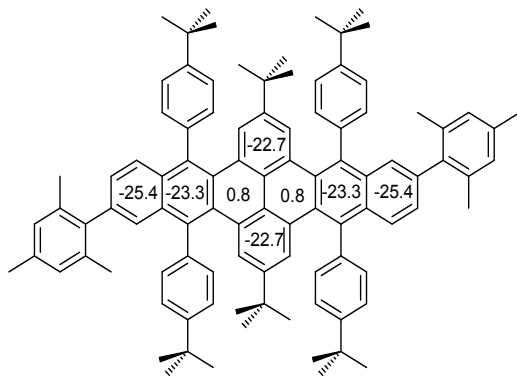
Optimized structure



LUMO = -1.45 eV

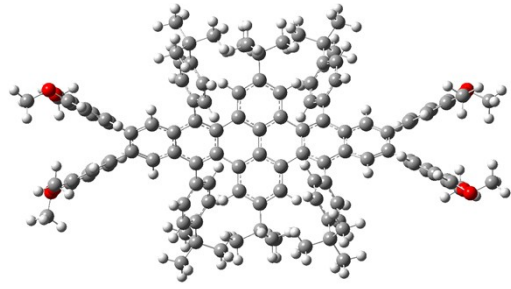


HOMO = -5.01 eV

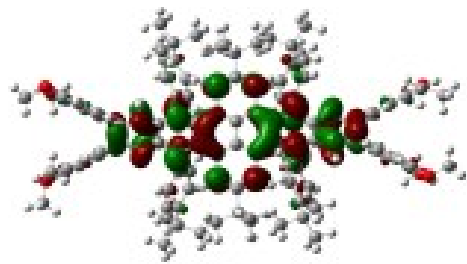


NICS(1)zz

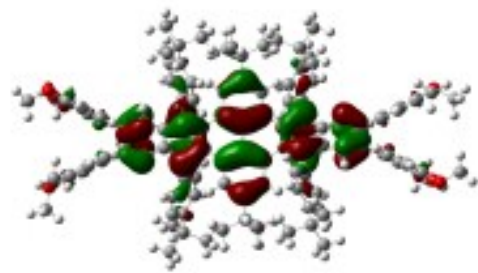
**3f**



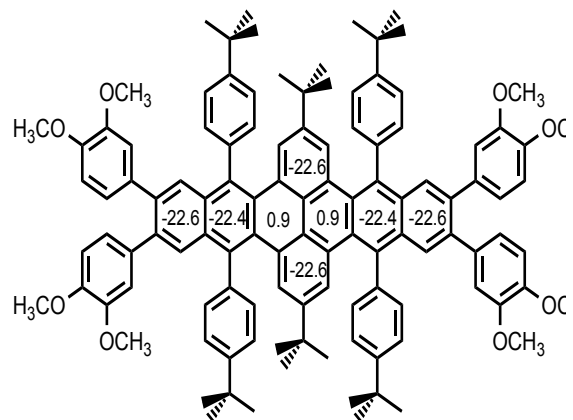
Optimized structure



LUMO = -1.51 eV



HOMO = -4.97 eV



NICS(1)zz

C	5.0327	5.0898	10.5352	C	5.0327	5.0898	10.5352
H	5.05366	6.08701	10.28685	H	5.06405	5.9083	10.04875
C	6.262	4.5539	11.034	C	6.262	4.5539	11.034
C	6.2043	3.6924	12.1764	C	6.2043	3.6924	12.1764
C	4.9378	3.2485	12.6422	C	4.9378	3.2485	12.6422
H	4.8927	2.6074	13.3157	H	4.8927	2.6074	13.3157
C	7.4282	3.3899	12.8594	C	7.4282	3.3899	12.8594
C	8.6435	3.87	12.3495	C	8.6435	3.87	12.3495
C	8.6879	4.3944	11.0136	C	8.6879	4.3944	11.0136
C	7.5106	4.8498	10.4203	C	7.5106	4.8498	10.4203
C	7.5133	5.7589	9.2386	C	7.5133	5.7589	9.2386
C	6.8853	5.4499	8.0426	C	6.8853	5.4499	8.0426
H	6.4584	4.6295	7.9466	H	6.4584	4.6295	7.9466
C	6.8845	6.3508	6.9773	C	6.8845	6.3508	6.9773
H	6.4534	6.1206	6.1874	H	6.4534	6.1206	6.1874
C	7.5162	7.5871	7.0749	C	7.5162	7.5871	7.0749
C	8.1416	7.8961	8.2897	C	8.1416	7.8961	8.2897
H	8.5613	8.7214	8.3872	H	8.5613	8.7214	8.3872
C	8.1488	7.0002	9.3519	C	8.1488	7.0002	9.3519
H	8.5823	7.2287	10.1434	H	8.5823	7.2287	10.1434
C	6.5889	9.7818	6.3683	C	6.5889	9.7818	6.3683
H	6.5511	10.4312	5.6618	H	6.5511	10.4312	5.6618
H	6.9474	10.1928	7.1598	H	6.9474	10.1928	7.1598
H	5.7055	9.4546	6.5493	H	5.7055	9.4546	6.5493
C	7.488	8.6195	5.9466	C	7.488	8.6195	5.9466
C	6.946	8.054	4.6421	C	6.946	8.054	4.6421
H	6.83	8.7642	4.0079	H	6.83	8.7642	4.0079
H	6.1017	7.6282	4.8042	H	6.1017	7.6282	4.8042
H	7.5655	7.4095	4.2912	H	7.5655	7.4095	4.2912
C	8.9036	9.1456	5.6665	C	8.9036	9.1456	5.6665
H	9.4739	8.414	5.4179	H	9.4739	8.414	5.4179
H	9.252	9.5648	6.4564	H	9.252	9.5648	6.4564
H	8.8747	9.7851	4.9521	H	8.8747	9.7851	4.9521
C	7.3848	2.5498	14.0852	C	7.3848	2.5498	14.0852
C	8.1839	1.4089	14.1906	C	8.1839	1.4089	14.1906
H	8.7242	1.1623	13.4747	H	8.7242	1.1623	13.4747

C	8.1883	0.6412	15.3394	C	8.1883	0.6412	15.3394
H	8.7388	-0.1085	15.3756	H	8.7388	-0.1085	15.3756
C	7.4004	0.9502	16.444	C	7.4004	0.9502	16.444
C	6.6152	2.0945	16.3528	C	6.6152	2.0945	16.3528
H	6.089	2.3443	17.0782	H	6.089	2.3443	17.0782
C	6.6004	2.8737	15.204	C	6.6004	2.8737	15.204
H	6.0593	3.63	15.1741	H	6.0593	3.63	15.1741
C	7.3605	0.0543	17.6809	C	7.3605	0.0543	17.6809
C	8.7078	-0.5458	17.9704	C	8.7078	-0.5458	17.9704
H	9.2686	0.1151	18.3827	H	9.2686	0.1151	18.3827
H	9.1087	-0.8401	17.1506	H	9.1087	-0.8401	17.1506
H	8.6025	-1.2938	18.5637	H	8.6025	-1.2938	18.5637
C	6.4419	-1.1656	17.3599	C	6.4419	-1.1656	17.3599
H	6.4456	-1.7739	18.1042	H	6.4456	-1.7739	18.1042
H	6.7696	-1.6161	16.5794	H	6.7696	-1.6161	16.5794
H	5.548	-0.8598	17.2009	H	5.548	-0.8598	17.2009
C	6.6074	0.7151	18.8453	C	6.6074	0.7151	18.8453
H	7.1687	1.3777	19.2545	H	7.1687	1.3777	19.2545
H	6.3745	0.0477	19.4952	H	6.3745	0.0477	19.4952
H	5.8093	1.1311	18.5149	H	5.8093	1.1311	18.5149
C	10.0028	4.3517	10.3243	C	10.0028	4.3517	10.3243
C	11.1759	4.1462	11.0797	C	11.1759	4.1462	11.0797
C	12.4265	3.9883	10.4392	C	12.4265	3.9883	10.4392
C	12.4732	4.1264	9.0497	C	12.4732	4.1264	9.0497
H	13.2989	4.087	8.6249	H	13.2989	4.087	8.6249
C	11.3343	4.3204	8.2787	C	11.3343	4.3204	8.2787
C	10.111	4.3845	8.9286	C	10.111	4.3845	8.9286
H	9.3346	4.452	8.4203	H	9.3346	4.452	8.4203
C	11.432	4.4158	6.746	C	11.432	4.4158	6.746
C	11.2171	3.0135	6.2015	C	11.2171	3.0135	6.2015
H	12.0675	2.5942	6.0505	H	12.0675	2.5942	6.0505
H	10.735	3.0611	5.3722	H	10.735	3.0611	5.3722
H	10.715	2.4956	6.8357	H	10.715	2.4956	6.8357
C	12.7193	4.863	6.2881	C	12.7193	4.863	6.2881
H	12.8102	5.8033	6.4564	H	12.8102	5.8033	6.4564
H	12.7974	4.6969	5.3455	H	12.7974	4.6969	5.3455

H	13.4088	4.3845	6.7554	H	13.4088	4.3845	6.7554
C	10.3702	5.2937	6.159	C	10.3702	5.2937	6.159
H	10.3871	6.1502	6.5933	H	10.3871	6.1502	6.5933
H	9.5102	4.886	6.2881	H	9.5102	4.886	6.2881
H	10.5306	5.4071	5.2196	H	10.5306	5.4071	5.2196
C	17.2512	5.0898	13.0687	C	17.2512	5.0898	13.0687
H	17.23038	6.087	13.31697	H	17.21997	5.9083	13.55506
C	16.0219	4.5539	12.5698	C	16.0219	4.5539	12.5698
C	16.0796	3.6924	11.4274	C	16.0796	3.6924	11.4274
C	17.3462	3.2485	10.9616	C	17.3462	3.2485	10.9616
H	17.3913	2.6074	10.2881	H	17.3913	2.6074	10.2881
C	14.8557	3.3899	10.7445	C	14.8557	3.3899	10.7445
C	13.6404	3.87	11.2543	C	13.6404	3.87	11.2543
C	13.5961	4.3944	12.5903	C	13.5961	4.3944	12.5903
C	14.7733	4.8498	13.1835	C	14.7733	4.8498	13.1835
C	14.7707	5.7589	14.3653	C	14.7707	5.7589	14.3653
C	15.3987	5.4499	15.5612	C	15.3987	5.4499	15.5612
H	15.8256	4.6295	15.6572	H	15.8256	4.6295	15.6572
C	15.3994	6.3508	16.6266	C	15.3994	6.3508	16.6266
H	15.8306	6.1206	17.4165	H	15.8306	6.1206	17.4165
C	14.7677	7.5871	16.529	C	14.7677	7.5871	16.529
C	14.1424	7.8961	15.3142	C	14.1424	7.8961	15.3142
H	13.7227	8.7214	15.2166	H	13.7227	8.7214	15.2166
C	14.1352	7.0002	14.252	C	14.1352	7.0002	14.252
H	13.7017	7.2287	13.4605	H	13.7017	7.2287	13.4605
C	15.6951	9.7818	17.2355	C	15.6951	9.7818	17.2355
H	15.7329	10.4312	17.9421	H	15.7329	10.4312	17.9421
H	15.3366	10.1928	16.444	H	15.3366	10.1928	16.444
H	16.5784	9.4546	17.0546	H	16.5784	9.4546	17.0546
C	14.796	8.6195	17.6573	C	14.796	8.6195	17.6573
C	15.3379	8.054	18.9618	C	15.3379	8.054	18.9618
H	15.4539	8.7642	19.5959	H	15.4539	8.7642	19.5959
H	16.1822	7.6282	18.7997	H	16.1822	7.6282	18.7997
H	14.7185	7.4095	19.3127	H	14.7185	7.4095	19.3127
C	13.3804	9.1456	17.9374	C	13.3804	9.1456	17.9374
H	12.8101	8.414	18.186	H	12.8101	8.414	18.186



H	13.032	9.5648	17.1474	H	13.032	9.5648	17.1474
H	13.4093	9.7851	18.6518	H	13.4093	9.7851	18.6518
C	14.8992	2.5498	9.5187	C	14.8992	2.5498	9.5187
C	14.1001	1.4089	9.4132	C	14.1001	1.4089	9.4132
H	13.5598	1.1623	10.1292	H	13.5598	1.1623	10.1292
C	14.0956	0.6412	8.2645	C	14.0956	0.6412	8.2645
H	13.5451	-0.1085	8.2283	H	13.5451	-0.1085	8.2283
C	14.8836	0.9502	7.1598	C	14.8836	0.9502	7.1598
C	15.6688	2.0945	7.2511	C	15.6688	2.0945	7.2511
H	16.195	2.3443	6.5257	H	16.195	2.3443	6.5257
C	15.6836	2.8737	8.3998	C	15.6836	2.8737	8.3998
H	16.2247	3.63	8.4297	H	16.2247	3.63	8.4297
C	14.9235	0.0543	5.923	C	14.9235	0.0543	5.923
C	13.5761	-0.5458	5.6335	C	13.5761	-0.5458	5.6335
H	13.0154	0.1151	5.2212	H	13.0154	0.1151	5.2212
H	13.1753	-0.8401	6.4533	H	13.1753	-0.8401	6.4533
H	13.6815	-1.2938	5.0402	H	13.6815	-1.2938	5.0402
C	15.842	-1.1656	6.244	C	15.842	-1.1656	6.244
H	15.8384	-1.7739	5.4997	H	15.8384	-1.7739	5.4997
H	15.5143	-1.6161	7.0245	H	15.5143	-1.6161	7.0245
H	16.736	-0.8598	6.4029	H	16.736	-0.8598	6.4029
C	15.6766	0.7151	4.7585	C	15.6766	0.7151	4.7585
H	15.1153	1.3777	4.3494	H	15.1153	1.3777	4.3494
H	15.9095	0.0477	4.1086	H	15.9095	0.0477	4.1086
H	16.4747	1.1311	5.089	H	16.4747	1.1311	5.089
C	12.2812	4.3517	13.2795	C	12.2812	4.3517	13.2795
C	11.1081	4.1462	12.5242	C	11.1081	4.1462	12.5242
C	9.8575	3.9883	13.1647	C	9.8575	3.9883	13.1647
C	9.8107	4.1264	14.5541	C	9.8107	4.1264	14.5541
H	8.9851	4.087	14.979	H	8.9851	4.087	14.979
C	10.9497	4.3204	15.3252	C	10.9497	4.3204	15.3252
C	12.173	4.3845	14.6753	C	12.173	4.3845	14.6753
H	12.9493	4.452	15.1836	H	12.9493	4.452	15.1836
C	10.852	4.4158	16.8579	C	10.852	4.4158	16.8579
C	11.0669	3.0135	17.4023	C	11.0669	3.0135	17.4023
H	10.2165	2.5942	17.5534	H	10.2165	2.5942	17.5534

H	11.549	3.0611	18.2316	H	11.549	3.0611	18.2316
H	11.5689	2.4956	16.7682	H	11.5689	2.4956	16.7682
C	9.5647	4.863	17.3158	C	9.5647	4.863	17.3158
H	9.4738	5.8033	17.1474	H	9.4738	5.8033	17.1474
H	9.4865	4.6969	18.2584	H	9.4865	4.6969	18.2584
H	8.8752	4.3845	16.8484	H	8.8752	4.3845	16.8484
C	11.9138	5.2937	17.4448	C	11.9138	5.2937	17.4448
H	11.8968	6.1502	17.0105	H	11.8968	6.1502	17.0105
H	12.7738	4.886	17.3158	H	12.7738	4.886	17.3158
H	11.7534	5.4071	18.3843	H	11.7534	5.4071	18.3843
C	3.7752	3.7582	12.1056	C	2.9075	5.17502	10.69139
H	3.33684	2.82721	11.15163	C	2.20992	4.57054	9.64567
C	18.5087	3.7582	11.4982	C	2.43769	6.3653	11.2472
H	18.94624	2.82585	12.4513	H	2.57996	3.63222	9.20777
C	2.9075	5.17502	10.69139	C	1.27085	6.95134	10.75671
C	2.46234	4.87174	9.40477	H	2.98769	6.84146	12.07197
C	2.18518	6.06386	11.48803	H	0.72478	7.70461	11.39058
C	1.2949	5.4575	8.91441	C	2.80992	3.40431	12.49564
C	1.01827	6.64988	10.99768	C	2.17704	2.31109	11.90412
C	0.57322	6.34684	9.71031	C	2.21849	4.04859	13.58262
H	0.94463	5.21878	7.89973	C	0.95243	1.86212	12.3993
H	0.44906	7.35108	11.62506	H	2.64329	1.80304	11.0476
C	3.84434	4.71856	11.07051	H	2.71791	4.91026	14.04906
C	3.25933	3.89026	8.5255	H	0.30014	1.21598	11.74778
H	4.08105	4.40412	8.07205	C	3.8275	4.7133	11.0781
H	3.62971	3.08929	9.13062	C	3.7752	3.7582	12.1056
H	2.62098	3.49544	7.76292	C	0.36056	2.50669	13.48532
C	2.6767	6.398	12.90872	C	0.57327	6.34685	9.7102
H	2.66389	5.51179	13.5082	O	-0.62268	6.94742	9.20628
H	3.67452	6.78124	12.85998	O	-0.89524	2.0467	13.99156
H	2.0332	7.13311	13.34508	C	-1.76089	6.28551	9.76418
C	-0.71495	6.99415	9.16881	H	-1.7447	5.25249	9.4858
H	-1.55382	6.64701	9.73511	H	-1.73421	6.36797	10.83066
H	-0.64259	8.05826	9.25437	H	-2.65544	6.74081	9.39351
H	-0.84346	6.72691	8.14072	C	-1.92317	2.31588	13.03458
C	19.37653	5.17495	12.91253	H	-1.98776	3.37082	12.86773

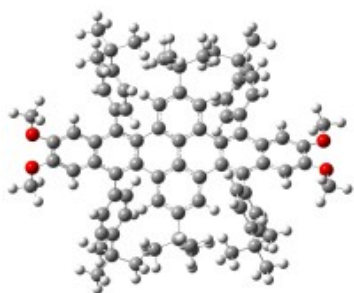
C	19.82283	4.86994	14.19835	H	-1.69125	1.82269	12.11378
C	20.09774	6.06543	12.11673	H	-2.85964	1.95556	13.40617
C	20.99029	5.45561	14.68874	O	0.56202	4.7403	8.43592
C	21.26467	6.65137	12.60711	O	0.58717	4.04376	14.82529
C	21.71086	6.3466	13.89367	C	1.04253	5.15641	9.15533
H	21.34147	5.21553	15.70278	C	0.99393	3.60007	14.07743
H	21.83302	7.35387	11.98039	C	1.43287	3.85134	7.73145
C	18.45144	4.8059	12.62543	H	2.3733	4.33289	7.56234
C	19.60496	6.40148	10.69692	H	1.58495	2.96595	8.31272
H	19.6104	5.51464	10.09827	H	0.99197	3.59001	6.79219
H	18.60983	6.79141	10.74773	C	1.56347	4.84867	15.49151
H	20.25226	7.13189	10.25828	H	2.45562	4.277	15.64037
C	19.02706	3.88665	15.0767	H	1.78587	5.70759	14.89343
H	18.20931	4.40089	15.53685	H	1.17944	5.1637	16.43923
H	18.65104	3.08993	14.46945	C	19.37653	5.17495	12.91253
H	19.66794	3.48593	15.83406	C	20.07524	4.56926	13.95679
C	22.99907	6.99381	14.4352	C	19.84523	6.36636	12.35821
H	23.83794	6.64658	13.86897	H	19.70606	3.63005	14.39352
H	22.92681	8.05793	14.34959	C	21.0121	6.95231	12.84873
H	23.1275	6.72661	15.46331	H	19.29434	6.84348	11.53459
E(SCF) = -3796.18720819 a.u.				H	21.38145	7.89178	12.41253
E(zp)=-3794.468598 a.u.				C	19.47392	3.40428	11.10804
				C	20.1065	2.31061	11.69905
				C	20.06557	4.04895	10.02142
				C	21.33104	1.86159	11.20372
				H	19.64007	1.80223	12.55529
				H	19.56638	4.91098	9.55539
				H	21.82986	0.99981	11.67036
				C	18.4565	4.7133	12.5258
				C	18.5087	3.7582	11.4982
				O	22.51371	6.74973	14.2321
				O	22.76612	2.19773	9.7781
				C	21.71081	6.34661	13.89379
				C	21.92312	2.50657	10.11806
				C	23.64065	6.2503	13.5072
				H	24.53301	6.71616	13.86993

H	23.7109	5.19122	13.64248
H	23.52129	6.46984	12.46679
C	22.54075	1.21499	8.76404
H	22.04699	1.66929	7.93055
H	23.47837	0.80964	8.44553
H	21.92825	0.4307	9.15727
O	21.72395	4.7381	15.16557
O	21.69696	4.04436	8.77885
C	20.84722	3.86753	15.88554
H	19.90871	4.35681	16.04271
H	20.69227	2.97143	15.32173
H	21.28467	3.62296	16.83091
C	21.17437	5.37092	8.66924
H	20.16721	5.32899	8.31038
H	21.19134	5.84148	9.63007
H	21.77352	5.93492	7.98526
C	21.24266	5.15505	14.44717
C	21.29005	3.60039	9.52646

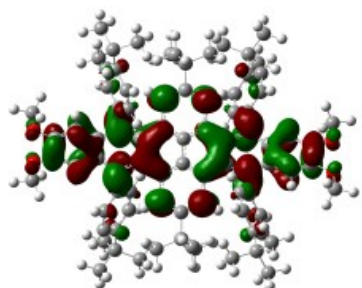
E(SCF) = -4938.56425451 a.u.

E(zp)=-4936.590374 a.u.

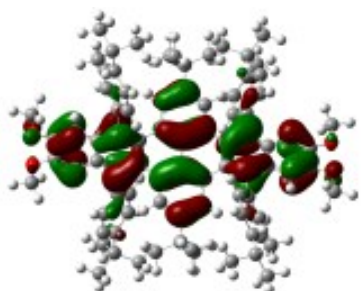
**3c**



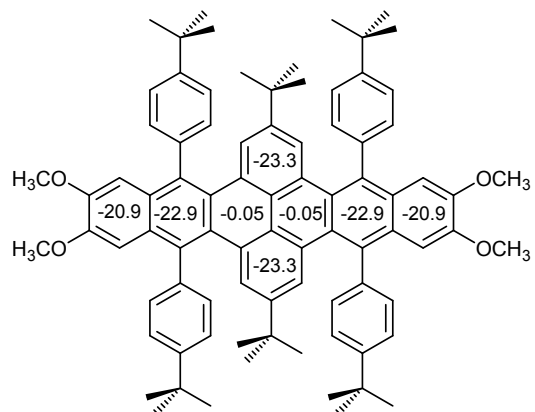
Optimized structure



LUMO = -1.17 eV

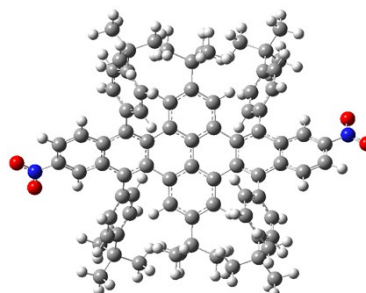


HOMO = -4.81 eV



NICS(1)zz

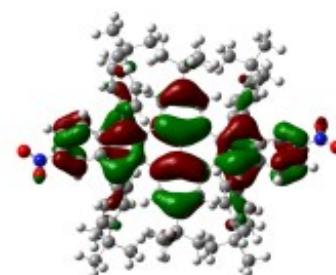
**3hx**



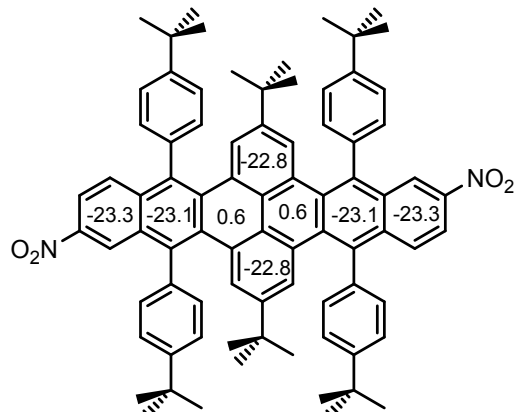
Optimized structure



LUMO = -2.40 eV



HOMO = -5.54 eV



NICS(1)zz

O	2.71216	5.48809	11.09337	C	5.0327	5.0898	10.5352
C	2.72922	6.63692	10.2619	H	5.06405	5.9083	10.04875
H	3.35221	7.27843	10.61183	C	6.262	4.5539	11.034
H	1.8523	7.02535	10.23541	C	6.2043	3.6924	12.1764
H	2.99491	6.38603	9.37287	C	4.9378	3.2485	12.6422
C	3.8275	4.7133	11.0781	H	4.8927	2.6074	13.3157
C	5.0327	5.0898	10.5352	C	7.4282	3.3899	12.8594
H	5.0501	5.7014	9.8349	C	8.6435	3.87	12.3495
C	6.262	4.5539	11.034	C	8.6879	4.3944	11.0136
C	6.2043	3.6924	12.1764	C	7.5106	4.8498	10.4203
C	4.9378	3.2485	12.6422	C	7.5133	5.7589	9.2386
H	4.87925	2.40386	13.09774	C	6.8853	5.4499	8.0426
C	7.4282	3.3899	12.8594	H	6.4584	4.6295	7.9466
C	8.6435	3.87	12.3495	C	6.8845	6.3508	6.9773
C	8.6879	4.3944	11.0136	H	6.4534	6.1206	6.1874
C	7.5106	4.8498	10.4203	C	7.5162	7.5871	7.0749
C	7.5133	5.7589	9.2386	C	8.1416	7.8961	8.2897
C	6.8853	5.4499	8.0426	H	8.5613	8.7214	8.3872
H	6.4584	4.6295	7.9466	C	8.1488	7.0002	9.3519
C	6.8845	6.3508	6.9773	H	8.5823	7.2287	10.1434
H	6.4534	6.1206	6.1874	C	6.5889	9.7818	6.3683
C	7.5162	7.5871	7.0749	H	6.5511	10.4312	5.6618
C	8.1416	7.8961	8.2897	H	6.9474	10.1928	7.1598
H	8.5613	8.7214	8.3872	H	5.7055	9.4546	6.5493
C	8.1488	7.0002	9.3519	C	7.488	8.6195	5.9466
H	8.5823	7.2287	10.1434	C	6.946	8.054	4.6421
C	6.5889	9.7818	6.3683	H	6.83	8.7642	4.0079
H	6.5511	10.4312	5.6618	H	6.1017	7.6282	4.8042
H	6.9474	10.1928	7.1598	H	7.5655	7.4095	4.2912
H	5.7055	9.4546	6.5493	C	8.9036	9.1456	5.6665
C	7.488	8.6195	5.9466	H	9.4739	8.414	5.4179
C	6.946	8.054	4.6421	H	9.252	9.5648	6.4564
H	6.83	8.7642	4.0079	H	8.8747	9.7851	4.9521
H	6.1017	7.6282	4.8042	C	7.3848	2.5498	14.0852
H	7.5655	7.4095	4.2912	C	8.1839	1.4089	14.1906
C	8.9036	9.1456	5.6665	H	8.7242	1.1623	13.4747

H	9.4739	8.414	5.4179	C	8.1883	0.6412	15.3394
H	9.252	9.5648	6.4564	H	8.7388	-0.1085	15.3756
H	8.8747	9.7851	4.9521	C	7.4004	0.9502	16.444
C	7.3848	2.5498	14.0852	C	6.6152	2.0945	16.3528
C	8.1839	1.4089	14.1906	H	6.089	2.3443	17.0782
H	8.7242	1.1623	13.4747	C	6.6004	2.8737	15.204
C	8.1883	0.6412	15.3394	H	6.0593	3.63	15.1741
H	8.7388	-0.1085	15.3756	C	7.3605	0.0543	17.6809
C	7.4004	0.9502	16.444	C	8.7078	-0.5458	17.9704
C	6.6152	2.0945	16.3528	H	9.2686	0.1151	18.3827
H	6.089	2.3443	17.0782	H	9.1087	-0.8401	17.1506
C	6.6004	2.8737	15.204	H	8.6025	-1.2938	18.5637
H	6.0593	3.63	15.1741	C	6.4419	-1.1656	17.3599
C	7.3605	0.0543	17.6809	H	6.4456	-1.7739	18.1042
C	8.7078	-0.5458	17.9704	H	6.7696	-1.6161	16.5794
H	9.2686	0.1151	18.3827	H	5.548	-0.8598	17.2009
H	9.1087	-0.8401	17.1506	C	6.6074	0.7151	18.8453
H	8.6025	-1.2938	18.5637	H	7.1687	1.3777	19.2545
C	6.4419	-1.1656	17.3599	H	6.3745	0.0477	19.4952
H	6.4456	-1.7739	18.1042	H	5.8093	1.1311	18.5149
H	6.7696	-1.6161	16.5794	C	10.0028	4.3517	10.3243
H	5.548	-0.8598	17.2009	C	11.1759	4.1462	11.0797
C	6.6074	0.7151	18.8453	C	12.4265	3.9883	10.4392
H	7.1687	1.3777	19.2545	C	12.4732	4.1264	9.0497
H	6.3745	0.0477	19.4952	H	13.2989	4.087	8.6249
H	5.8093	1.1311	18.5149	C	11.3343	4.3204	8.2787
C	10.0028	4.3517	10.3243	C	10.111	4.3845	8.9286
C	11.1759	4.1462	11.0797	H	9.3346	4.452	8.4203
C	12.4265	3.9883	10.4392	C	11.432	4.4158	6.746
C	12.4732	4.1264	9.0497	C	11.2171	3.0135	6.2015
H	13.2989	4.087	8.6249	H	12.0675	2.5942	6.0505
C	11.3343	4.3204	8.2787	H	10.735	3.0611	5.3722
C	10.111	4.3845	8.9286	H	10.715	2.4956	6.8357
H	9.3346	4.452	8.4203	C	12.7193	4.863	6.2881
C	11.432	4.4158	6.746	H	12.8102	5.8033	6.4564
C	11.2171	3.0135	6.2015	H	12.7974	4.6969	5.3455

H	12.0675	2.5942	6.0505	H	13.4088	4.3845	6.7554
H	10.735	3.0611	5.3722	C	10.3702	5.2937	6.159
H	10.715	2.4956	6.8357	H	10.3871	6.1502	6.5933
C	12.7193	4.863	6.2881	H	9.5102	4.886	6.2881
H	12.8102	5.8033	6.4564	H	10.5306	5.4071	5.2196
H	12.7974	4.6969	5.3455	C	17.2512	5.0898	13.0687
H	13.4088	4.3845	6.7554	H	17.21997	5.9083	13.55506
C	10.3702	5.2937	6.159	C	16.0219	4.5539	12.5698
H	10.3871	6.1502	6.5933	C	16.0796	3.6924	11.4274
H	9.5102	4.886	6.2881	C	17.3462	3.2485	10.9616
H	10.5306	5.4071	5.2196	H	17.3913	2.6074	10.2881
O	19.57182	5.48812	12.51054	C	14.8557	3.3899	10.7445
C	19.55464	6.63692	13.34192	C	13.6404	3.87	11.2543
H	18.93174	7.27844	12.99209	C	13.5961	4.3944	12.5903
H	20.43166	7.02538	13.3685	C	14.7733	4.8498	13.1835
H	19.28907	6.38603	14.23104	C	14.7707	5.7589	14.3653
C	18.4565	4.7133	12.5258	C	15.3987	5.4499	15.5612
C	17.2512	5.0898	13.0687	H	15.8256	4.6295	15.6572
H	17.2339	5.7014	13.7689	C	15.3994	6.3508	16.6266
C	16.0219	4.5539	12.5698	H	15.8306	6.1206	17.4165
C	16.0796	3.6924	11.4274	C	14.7677	7.5871	16.529
C	17.3462	3.2485	10.9616	C	14.1424	7.8961	15.3142
H	17.40477	2.40386	10.50605	H	13.7227	8.7214	15.2166
C	14.8557	3.3899	10.7445	C	14.1352	7.0002	14.252
C	13.6404	3.87	11.2543	H	13.7017	7.2287	13.4605
C	13.5961	4.3944	12.5903	C	15.6951	9.7818	17.2355
C	14.7733	4.8498	13.1835	H	15.7329	10.4312	17.9421
C	14.7707	5.7589	14.3653	H	15.3366	10.1928	16.444
C	15.3987	5.4499	15.5612	H	16.5784	9.4546	17.0546
H	15.8256	4.6295	15.6572	C	14.796	8.6195	17.6573
C	15.3994	6.3508	16.6266	C	15.3379	8.054	18.9618
H	15.8306	6.1206	17.4165	H	15.4539	8.7642	19.5959
C	14.7677	7.5871	16.529	H	16.1822	7.6282	18.7997
C	14.1424	7.8961	15.3142	H	14.7185	7.4095	19.3127
H	13.7227	8.7214	15.2166	C	13.3804	9.1456	17.9374
C	14.1352	7.0002	14.252	H	12.8101	8.414	18.186



H	13.7017	7.2287	13.4605	H	13.032	9.5648	17.1474
C	15.6951	9.7818	17.2355	H	13.4093	9.7851	18.6518
H	15.7329	10.4312	17.9421	C	14.8992	2.5498	9.5187
H	15.3366	10.1928	16.444	C	14.1001	1.4089	9.4132
H	16.5784	9.4546	17.0546	H	13.5598	1.1623	10.1292
C	14.796	8.6195	17.6573	C	14.0956	0.6412	8.2645
C	15.3379	8.054	18.9618	H	13.5451	-0.1085	8.2283
H	15.4539	8.7642	19.5959	C	14.8836	0.9502	7.1598
H	16.1822	7.6282	18.7997	C	15.6688	2.0945	7.2511
H	14.7185	7.4095	19.3127	H	16.195	2.3443	6.5257
C	13.3804	9.1456	17.9374	C	15.6836	2.8737	8.3998
H	12.8101	8.414	18.186	H	16.2247	3.63	8.4297
H	13.032	9.5648	17.1474	C	14.9235	0.0543	5.923
H	13.4093	9.7851	18.6518	C	13.5761	-0.5458	5.6335
C	14.8992	2.5498	9.5187	H	13.0154	0.1151	5.2212
C	14.1001	1.4089	9.4132	H	13.1753	-0.8401	6.4533
H	13.5598	1.1623	10.1292	H	13.6815	-1.2938	5.0402
C	14.0956	0.6412	8.2645	C	15.842	-1.1656	6.244
H	13.5451	-0.1085	8.2283	H	15.8384	-1.7739	5.4997
C	14.8836	0.9502	7.1598	H	15.5143	-1.6161	7.0245
C	15.6688	2.0945	7.2511	H	16.736	-0.8598	6.4029
H	16.195	2.3443	6.5257	C	15.6766	0.7151	4.7585
C	15.6836	2.8737	8.3998	H	15.1153	1.3777	4.3494
H	16.2247	3.63	8.4297	H	15.9095	0.0477	4.1086
C	14.9235	0.0543	5.923	H	16.4747	1.1311	5.089
C	13.5761	-0.5458	5.6335	C	12.2812	4.3517	13.2795
H	13.0154	0.1151	5.2212	C	11.1081	4.1462	12.5242
H	13.1753	-0.8401	6.4533	C	9.8575	3.9883	13.1647
H	13.6815	-1.2938	5.0402	C	9.8107	4.1264	14.5541
C	15.842	-1.1656	6.244	H	8.9851	4.087	14.979
H	15.8384	-1.7739	5.4997	C	10.9497	4.3204	15.3252
H	15.5143	-1.6161	7.0245	C	12.173	4.3845	14.6753
H	16.736	-0.8598	6.4029	H	12.9493	4.452	15.1836
C	15.6766	0.7151	4.7585	C	10.852	4.4158	16.8579
H	15.1153	1.3777	4.3494	C	11.0669	3.0135	17.4023
H	15.9095	0.0477	4.1086	H	10.2165	2.5942	17.5534

H	16.4747	1.1311	5.089	H	11.549	3.0611	18.2316
C	12.2812	4.3517	13.2795	H	11.5689	2.4956	16.7682
C	11.1081	4.1462	12.5242	C	9.5647	4.863	17.3158
C	9.8575	3.9883	13.1647	H	9.4738	5.8033	17.1474
C	9.8107	4.1264	14.5541	H	9.4865	4.6969	18.2584
H	8.9851	4.087	14.979	H	8.8752	4.3845	16.8484
C	10.9497	4.3204	15.3252	C	11.9138	5.2937	17.4448
C	12.173	4.3845	14.6753	H	11.8968	6.1502	17.0105
H	12.9493	4.452	15.1836	H	12.7738	4.886	17.3158
C	10.852	4.4158	16.8579	H	11.7534	5.4071	18.3843
C	11.0669	3.0135	17.4023	C	3.7752	3.7582	12.1056
H	10.2165	2.5942	17.5534	H	3.25201	2.88112	11.41781
H	11.549	3.0611	18.2316	C	18.5087	3.7582	11.4982
H	11.5689	2.4956	16.7682	H	19.03108	2.87984	12.18502
C	9.5647	4.863	17.3158	N	2.95097	5.1532	10.70967
H	9.4738	5.8033	17.1474	O	2.51219	4.76168	9.66439
H	9.4865	4.6969	18.2584	O	2.43544	6.02366	11.35382
H	8.8752	4.3845	16.8484	N	19.33305	5.15313	12.89425
C	11.9138	5.2937	17.4448	O	19.76511	4.76996	13.94541
H	11.8968	6.1502	17.0105	O	19.85534	6.01518	12.24425
H	12.7738	4.886	17.3158	C	18.4565	4.7133	12.5258
H	11.7534	5.4071	18.3843	C	3.8275	4.7133	11.0781
C	2.99242	2.24664	13.44228				
H	2.01206	1.88686	13.83879				
H	3.49265	1.3937	12.92233				
H	3.62942	2.54898	14.30882				
O	2.79453	3.39867	12.50186				
C	19.29403	2.22513	10.18776				
H	20.27433	1.86532	9.79114				
H	18.80531	1.37928	10.72976				
H	18.64765	2.50348	9.32013				
O	19.48931	3.39864	11.10182				
C	18.5087	3.7582	11.4982				
C	3.7752	3.7582	12.1056				

E(SCF)=-3507.15414794 a.u.

E(zp)=-3505.757033 a.u.

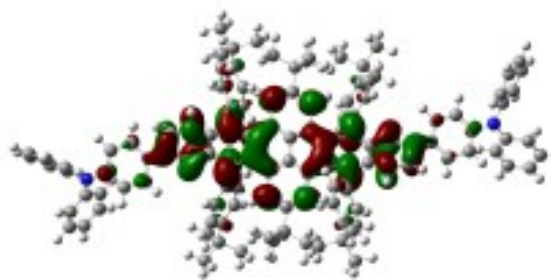
E(SCF)=-3556.24434104 a.u.

E(zp)=-3554.722276 a.u.

**3l**



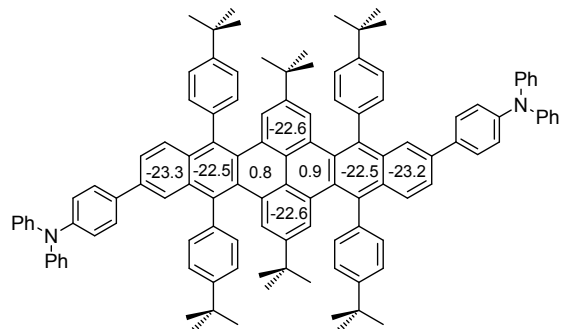
Optimized structure



LUMO = -1.49 eV



HOMO = -4.77 eV



NICS(1)zz

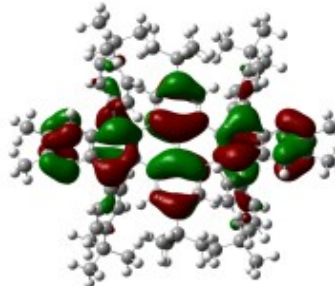
**3b**



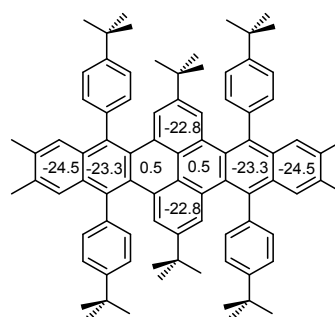
Optimized structure



LUMO = -1.31 eV



HOMO = -4.89 eV



NICS(1)zz

C	5.0327	5.0898	0.5352	C	3.8275	4.7133	11.0781
H	5.06405	5.9083	10.04875	C	5.0327	5.0898	10.5352
C	6.262	4.5539	11.034	H	5.0501	5.7014	9.8349
C	6.2043	3.6924	12.1764	C	6.262	4.5539	11.034
C	4.9378	3.2485	12.6422	C	6.2043	3.6924	12.1764
H	4.8927	2.6074	13.3157	C	4.9378	3.2485	12.6422
C	7.4282	3.3899	12.8594	H	4.8927	2.6074	13.3157
C	8.6435	3.87	12.3495	C	7.4282	3.3899	12.8594
C	8.6879	4.3944	11.0136	C	8.6435	3.87	12.3495
C	7.5106	4.8498	10.4203	C	8.6879	4.3944	11.0136
C	7.5133	5.7589	9.2386	C	7.5106	4.8498	10.4203
C	6.8853	5.4499	8.0426	C	7.5133	5.7589	9.2386
H	6.4584	4.6295	7.9466	C	6.8853	5.4499	8.0426
C	6.8845	6.3508	6.9773	H	6.4584	4.6295	7.9466
H	6.4534	6.1206	6.1874	C	6.8845	6.3508	6.9773
C	7.5162	7.5871	7.0749	H	6.4534	6.1206	6.1874
C	8.1416	7.8961	8.2897	C	7.5162	7.5871	7.0749
H	8.5613	8.7214	8.3872	C	8.1416	7.8961	8.2897
C	8.1488	7.0002	9.3519	H	8.5613	8.7214	8.3872
H	8.5823	7.2287	10.1434	C	8.1488	7.0002	9.3519
C	6.5889	9.7818	6.3683	H	8.5823	7.2287	10.1434
H	6.5511	10.4312	5.6618	C	6.5889	9.7818	6.3683
H	6.9474	10.1928	7.1598	H	6.5511	10.4312	5.6618
H	5.7055	9.4546	6.5493	H	6.9474	10.1928	7.1598
C	7.488	8.6195	5.9466	H	5.7055	9.4546	6.5493
C	6.946	8.054	4.6421	C	7.488	8.6195	5.9466
H	6.83	8.7642	4.0079	C	6.946	8.054	4.6421
H	6.1017	7.6282	4.8042	H	6.83	8.7642	4.0079
H	7.5655	7.4095	4.2912	H	6.1017	7.6282	4.8042
C	8.9036	9.1456	5.6665	H	7.5655	7.4095	4.2912
H	9.4739	8.414	5.4179	C	8.9036	9.1456	5.6665
H	9.252	9.5648	6.4564	H	9.4739	8.414	5.4179
H	8.8747	9.7851	4.9521	H	9.252	9.5648	6.4564
C	7.3848	2.5498	14.0852	H	8.8747	9.7851	4.9521
C	8.1839	1.4089	14.1906	C	7.3848	2.5498	14.0852

H	8.7242	1.1623	13.4747	C	8.1839	1.4089	14.1906
C	8.1883	0.6412	15.3394	H	8.7242	1.1623	13.4747
H	8.7388	-0.1085	15.3756	C	8.1883	0.6412	15.3394
C	7.4004	0.9502	16.444	H	8.7388	-0.1085	15.3756
C	6.6152	2.0945	16.3528	C	7.4004	0.9502	16.444
H	6.089	2.3443	17.0782	C	6.6152	2.0945	16.3528
C	6.6004	2.8737	15.204	H	6.089	2.3443	17.0782
H	6.0593	3.63	15.1741	C	6.6004	2.8737	15.204
C	7.3605	0.0543	17.6809	H	6.0593	3.63	15.1741
C	8.7078	-0.5458	17.9704	C	7.3605	0.0543	17.6809
H	9.2686	0.1151	18.3827	C	8.7078	-0.5458	17.9704
H	9.1087	-0.8401	17.1506	H	9.2686	0.1151	18.3827
H	8.6025	-1.2938	18.5637	H	9.1087	-0.8401	17.1506
C	6.4419	-1.1656	17.3599	H	8.6025	-1.2938	18.5637
H	6.4456	-1.7739	18.1042	C	6.4419	-1.1656	17.3599
H	6.7696	-1.6161	16.5794	H	6.4456	-1.7739	18.1042
H	5.548	-0.8598	17.2009	H	6.7696	-1.6161	16.5794
C	6.6074	0.7151	18.8453	H	5.548	-0.8598	17.2009
H	7.1687	1.3777	19.2545	C	6.6074	0.7151	18.8453
H	6.3745	0.0477	19.4952	H	7.1687	1.3777	19.2545
H	5.8093	1.1311	18.5149	H	6.3745	0.0477	19.4952
C	10.0028	4.3517	10.3243	H	5.8093	1.1311	18.5149
C	11.1759	4.1462	11.0797	C	10.0028	4.3517	10.3243
C	12.4265	3.9883	10.4392	C	11.1759	4.1462	11.0797
C	12.4732	4.1264	9.0497	C	12.4265	3.9883	10.4392
H	13.2989	4.087	8.6249	C	12.4732	4.1264	9.0497
C	11.3343	4.3204	8.2787	H	13.2989	4.087	8.6249
C	10.111	4.3845	8.9286	C	11.3343	4.3204	8.2787
H	9.3346	4.452	8.4203	C	10.111	4.3845	8.9286
C	11.432	4.4158	6.746	H	9.3346	4.452	8.4203
C	11.2171	3.0135	6.2015	C	11.432	4.4158	6.746
H	12.0675	2.5942	6.0505	C	11.2171	3.0135	6.2015
H	10.735	3.0611	5.3722	H	12.0675	2.5942	6.0505
H	10.715	2.4956	6.8357	H	10.735	3.0611	5.3722
C	12.7193	4.863	6.2881	H	10.715	2.4956	6.8357
H	12.8102	5.8033	6.4564	C	12.7193	4.863	6.2881

H	12.7974	4.6969	5.3455	H	12.8102	5.8033	6.4564
H	13.4088	4.3845	6.7554	H	12.7974	4.6969	5.3455
C	10.3702	5.2937	6.159	H	13.4088	4.3845	6.7554
H	10.3871	6.1502	6.5933	C	10.3702	5.2937	6.159
H	9.5102	4.886	6.2881	H	10.3871	6.1502	6.5933
H	10.5306	5.4071	5.2196	H	9.5102	4.886	6.2881
C	17.2512	5.0898	13.0687	H	10.5306	5.4071	5.2196
H	17.21997	5.9083	13.55506	C	18.4565	4.7133	12.5258
C	16.0219	4.5539	12.5698	C	17.2512	5.0898	13.0687
C	16.0796	3.6924	11.4274	C	16.0219	4.5539	12.5698
C	17.3462	3.2485	10.9616	C	16.0796	3.6924	11.4274
H	17.3913	2.6074	10.2881	C	17.3462	3.2485	10.9616
C	14.8557	3.3899	10.7445	H	17.3913	2.6074	10.2881
C	13.6404	3.87	11.2543	C	14.8557	3.3899	10.7445
C	13.5961	4.3944	12.5903	C	13.6404	3.87	11.2543
C	14.7733	4.8498	13.1835	C	13.5961	4.3944	12.5903
C	14.7707	5.7589	14.3653	C	14.7733	4.8498	13.1835
C	15.3987	5.4499	15.5612	C	14.7707	5.7589	14.3653
H	15.8256	4.6295	15.6572	C	15.3987	5.4499	15.5612
C	15.3994	6.3508	16.6266	H	15.8256	4.6295	15.6572
H	15.8306	6.1206	17.4165	C	15.3994	6.3508	16.6266
C	14.7677	7.5871	16.529	H	15.8306	6.1206	17.4165
C	14.1424	7.8961	15.3142	C	14.7677	7.5871	16.529
H	13.7227	8.7214	15.2166	C	14.1424	7.8961	15.3142
C	14.1352	7.0002	14.252	H	13.7227	8.7214	15.2166
H	13.7017	7.2287	13.4605	C	14.1352	7.0002	14.252
C	15.6951	9.7818	17.2355	H	13.7017	7.2287	13.4605
H	15.7329	10.4312	17.9421	C	15.6951	9.7818	17.2355
H	15.3366	10.1928	16.444	H	15.7329	10.4312	17.9421
H	16.5784	9.4546	17.0546	H	15.3366	10.1928	16.444
C	14.796	8.6195	17.6573	H	16.5784	9.4546	17.0546
C	15.3379	8.054	18.9618	C	14.796	8.6195	17.6573
H	15.4539	8.7642	19.5959	C	15.3379	8.054	18.9618
H	16.1822	7.6282	18.7997	H	15.4539	8.7642	19.5959
H	14.7185	7.4095	19.3127	H	16.1822	7.6282	18.7997
C	13.3804	9.1456	17.9374	H	14.7185	7.4095	19.3127

H	12.8101	8.414	18.186	C	13.3804	9.1456	17.9374
H	13.032	9.5648	17.1474	H	12.8101	8.414	18.186
H	13.4093	9.7851	18.6518	H	13.032	9.5648	17.1474
C	14.8992	2.5498	9.5187	H	13.4093	9.7851	18.6518
C	14.1001	1.4089	9.4132	C	14.8992	2.5498	9.5187
H	13.5598	1.1623	10.1292	C	14.1001	1.4089	9.4132
C	14.0956	0.6412	8.2645	H	13.5598	1.1623	10.1292
H	13.5451	-0.1085	8.2283	C	14.0956	0.6412	8.2645
C	14.8836	0.9502	7.1598	H	13.5451	-0.1085	8.2283
C	15.6688	2.0945	7.2511	C	14.8836	0.9502	7.1598
H	16.195	2.3443	6.5257	C	15.6688	2.0945	7.2511
C	15.6836	2.8737	8.3998	H	16.195	2.3443	6.5257
H	16.2247	3.63	8.4297	C	15.6836	2.8737	8.3998
C	14.9235	0.0543	5.923	H	16.2247	3.63	8.4297
C	13.5761	-0.5458	5.6335	C	14.9235	0.0543	5.923
H	13.0154	0.1151	5.2212	C	13.5761	-0.5458	5.6335
H	13.1753	-0.8401	6.4533	H	13.0154	0.1151	5.2212
H	13.6815	-1.2938	5.0402	H	13.1753	-0.8401	6.4533
C	15.842	-1.1656	6.244	H	13.6815	-1.2938	5.0402
H	15.8384	-1.7739	5.4997	C	15.842	-1.1656	6.244
H	15.5143	-1.6161	7.0245	H	15.8384	-1.7739	5.4997
H	16.736	-0.8598	6.4029	H	15.5143	-1.6161	7.0245
C	15.6766	0.7151	4.7585	H	16.736	-0.8598	6.4029
H	15.1153	1.3777	4.3494	C	15.6766	0.7151	4.7585
H	15.9095	0.0477	4.1086	H	15.1153	1.3777	4.3494
H	16.4747	1.1311	5.089	H	15.9095	0.0477	4.1086
C	12.2812	4.3517	13.2795	H	16.4747	1.1311	5.089
C	11.1081	4.1462	12.5242	C	12.2812	4.3517	13.2795
C	9.8575	3.9883	13.1647	C	11.1081	4.1462	12.5242
C	9.8107	4.1264	14.5541	C	9.8575	3.9883	13.1647
H	8.9851	4.087	14.979	C	9.8107	4.1264	14.5541
C	10.9497	4.3204	15.3252	H	8.9851	4.087	14.979
C	12.173	4.3845	14.6753	C	10.9497	4.3204	15.3252
H	12.9493	4.452	15.1836	C	12.173	4.3845	14.6753
C	10.852	4.4158	16.8579	H	12.9493	4.452	15.1836
C	11.0669	3.0135	17.4023	C	10.852	4.4158	16.8579

H	10.2165	2.5942	17.5534	C	11.0669	3.0135	17.4023
H	11.549	3.0611	18.2316	H	10.2165	2.5942	17.5534
H	11.5689	2.4956	16.7682	H	11.549	3.0611	18.2316
C	9.5647	4.863	17.3158	H	11.5689	2.4956	16.7682
H	9.4738	5.8033	17.1474	C	9.5647	4.863	17.3158
H	9.4865	4.6969	18.2584	H	9.4738	5.8033	17.1474
H	8.8752	4.3845	16.8484	H	9.4865	4.6969	18.2584
C	11.9138	5.2937	17.4448	H	8.8752	4.3845	16.8484
H	11.8968	6.1502	17.0105	C	11.9138	5.2937	17.4448
H	12.7738	4.886	17.3158	H	11.8968	6.1502	17.0105
H	11.7534	5.4071	18.3843	H	12.7738	4.886	17.3158
C	3.7752	3.7582	12.1056	H	11.7534	5.4071	18.3843
H	3.25201	2.88112	11.41781	C	3.7752	3.7582	12.1056
C	18.5087	3.7582	11.4982	C	3.25201	2.88112	11.41781
H	19.03108	2.87984	12.18502	H	18.5087	3.7582	11.4982
C	19.37653	5.17495	12.91253	C	19.03108	2.87984	12.18502
C	19.91422	4.74788	14.12663	H	19.37653	5.17495	12.91253
C	20.00631	6.18759	12.18841	H	19.91422	4.74788	14.12663
C	21.08167	5.33359	14.61701	H	20.00631	6.18759	12.18841
H	19.41809	3.94952	14.69726	C	21.08167	5.33359	14.61701
C	21.17322	6.77353	12.67884	H	19.41809	3.94952	14.69726
H	19.58236	6.52383	11.23098	H	21.17322	6.77353	12.67884
C	21.71084	6.34661	13.89371	H	19.58236	6.52383	11.23098
H	21.50491	4.9972	15.57459	C	21.71084	6.34661	13.89371
H	21.66951	7.57224	12.1087	H	21.50491	4.9972	15.57459
N	22.94046	6.96439	14.41072	H	21.66951	7.57224	12.1087
C	23.62332	7.6808	13.32382	H	22.94046	6.96439	14.41072
C	23.46393	9.05994	13.18926	C	23.62332	7.6808	13.32382
C	24.43133	6.98119	12.42712	H	23.46393	9.05994	13.18926
C	24.1123	9.73972	12.15775	H	24.43133	6.98119	12.42712
H	22.82736	9.61148	13.89617	H	24.1123	9.73972	12.15775
C	25.07919	7.66066	11.39555	H	22.82736	9.61148	13.89617
H	24.55714	5.89386	12.5337	H	25.07919	7.66066	11.39555
C	24.91931	9.04032	11.26065	H	24.55714	5.89386	12.5337
H	23.98582	10.82689	12.05148	C	24.91931	9.04032	11.26065
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E(zp)=-3253.928632 a.u.



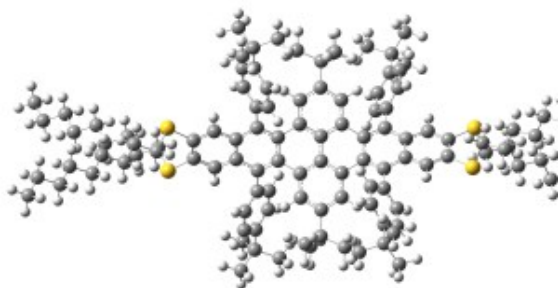
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C	25.0767	3.87554	14.62748
H	23.89162	4.81797	13.07925
C	25.10468	4.99057	16.7709
H	23.94243	6.81233	16.91188
C	25.51131	3.93692	15.95132
H	25.39668	3.04515	13.98149
H	25.44753	5.03879	17.81465
H	26.17462	3.15531	16.3493
C	2.9075	5.17502	10.69139
C	2.37096	4.74951	9.47623
C	2.27659	6.18617	11.4166
C	1.20354	5.33531	8.98588
H	2.86798	3.95232	8.90475
C	1.10971	6.77221	10.9262
H	2.69963	6.52118	12.37487
C	0.57324	6.34685	9.71027
H	0.78122	5.00016	8.02747
H	0.61253	7.56975	11.49721
C	3.8275	4.7133	11.0781
N	-0.65634	6.96472	9.19329
C	-1.52061	5.92612	8.61429
C	-2.28318	5.10845	9.44822
C	-1.57846	5.75866	7.23044
C	-3.10355	4.12294	8.89846
H	-2.23789	5.24059	10.53892
C	-2.39825	4.7731	6.68077
H	-0.97741	6.40378	6.57315
C	-3.16075	3.95475	7.51511
H	-3.70404	3.47796	9.55623
H	-2.44356	4.64034	5.59007
H	-3.80688	3.17757	7.08175
C	-1.36609	7.63676	10.29126

C	-1.85933	6.89177	11.36236
C	-1.54584	9.01996	10.26215
C	-2.53271	7.52982	12.40443
H	-1.7174	5.8016	11.38554
C	-2.21947	9.65787	11.3037
H	-1.15647	9.60714	9.4177
C	-2.71336	8.91247	12.37499
H	-2.92213	6.94211	13.24834
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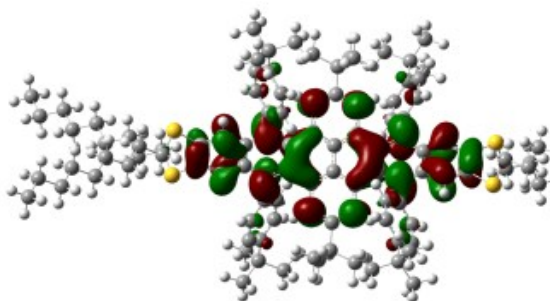
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E(zp) = -4593.295437 a.u.

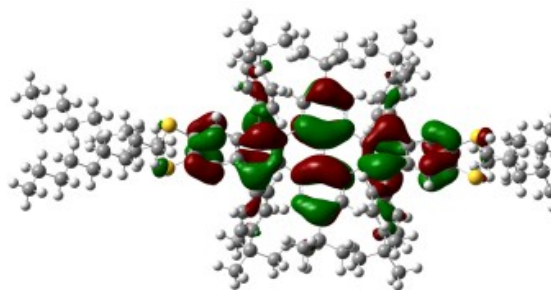
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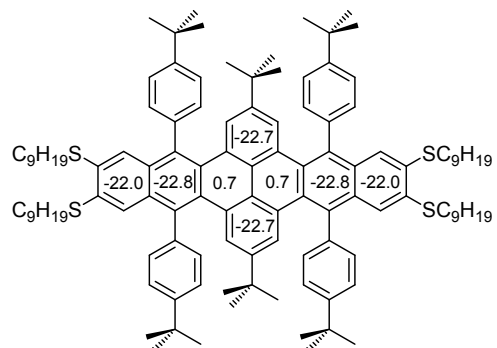
Optimized structure



LUMO = -1.63 eV



HOMO = -5.14 eV



NICS(1)zz

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H	-6.21692	-3.00303	-1.56681
C	-4.99959	-1.23871	-1.22974
C	-5.03887	0.19246	-1.21589
C	-6.30923	0.83663	-1.20953
H	-6.32624	1.91236	-1.12151
C	-3.8106	0.92465	-1.26578
C	-2.59373	0.22736	-1.1974
C	-2.59313	-1.16546	-0.8098
C	-3.76758	-1.91803	-0.97755
C	-3.76948	-3.41384	-0.99317
C	-4.55116	-4.18271	-0.11991
H	-5.1388	-3.68691	0.6475
C	-4.58716	-5.57579	-0.21394
H	-5.20733	-6.12055	0.48853
C	-3.85298	-6.26467	-1.18905
C	-3.0656	-5.4874	-2.05588
H	-2.48	-5.97104	-2.83203
C	-3.0202	-4.10025	-1.9619
H	-2.40667	-3.53336	-2.6554
C	-4.49238	-8.13783	-2.73843
H	-4.5348	-9.22398	-2.87794
H	-3.88996	-7.72036	-3.55064
H	-5.50818	-7.74216	-2.83949
C	-3.8994	-7.79468	-1.35056
C	-4.77009	-8.46964	-0.27396
H	-4.76744	-9.55388	-0.42467
H	-5.81128	-8.13442	-0.32067
H	-4.39246	-8.27543	0.73533
C	-2.47008	-8.3773	-1.24828
H	-2.02436	-8.15528	-0.27344
H	-1.80706	-7.9727	-2.01833
H	-2.49527	-9.46578	-1.37155
C	-3.87809	2.41879	-1.30565

C	-3.34065	3.17665	-0.25327
H	-2.84275	2.66633	0.5656
C	-3.44135	4.56437	-0.24169
H	-3.01606	5.10607	0.59812
C	-4.08168	5.27043	-1.27482
C	-4.61575	4.50947	-2.32401
H	-5.11655	4.99687	-3.1526
C	-4.51927	3.11632	-2.33898
H	-4.94279	2.56337	-3.17252
C	-4.18432	6.80511	-1.21234
C	-2.76699	7.41854	-1.12106
H	-2.16834	7.15564	-1.99922
H	-2.22836	7.07259	-0.23416
H	-2.82871	8.51121	-1.06706
C	-4.99764	7.21026	0.04036
H	-5.07404	8.30118	0.10987
H	-4.53104	6.84913	0.96158
H	-6.01241	6.80098	-0.00252
C	-4.88282	7.39549	-2.45159
H	-4.34414	7.1573	-3.37452
H	-4.92544	8.48603	-2.36622
H	-5.91113	7.03334	-2.55214
C	-1.36681	-1.67139	-0.15025
C	-0.15433	-0.9426	-0.27101
C	0.99582	-1.32691	0.45686
C	0.92941	-2.48142	1.25439
H	1.82388	-2.81589	1.75408
C	-0.25175	-3.20641	1.41028
C	-1.38822	-2.76957	0.71907
H	-2.31798	-3.29611	0.86991
C	-0.34922	-4.44472	2.32323
C	-1.34861	-4.15175	3.46789
H	-1.01445	-3.29981	4.06909
H	-1.43652	-5.02189	4.12865
H	-2.34771	-3.92148	3.08618
C	1.00488	-4.81955	2.95321

H	1.75437	-5.05922	2.19144
H	0.88156	-5.7072	3.58269
H	1.40377	-4.01881	3.58263
C	-0.84803	-5.65933	1.50654
H	-0.15372	-5.89291	0.69272
H	-1.83216	-5.48409	1.06548
H	-0.92294	-6.5423	2.15216
C	7.26984	0.1728	-0.29135
C	6.17682	0.23063	-1.13155
C	4.83603	0.10359	-0.66451
C	4.63892	-0.23815	0.71183
C	5.77027	-0.19442	1.57694
H	5.62384	-0.33125	2.64007
C	3.3423	-0.64065	1.15811
C	2.26678	-0.59578	0.25582
C	2.41303	0.12389	-0.98945
C	3.70269	0.33636	-1.50547
C	3.95258	0.7148	-2.93085
C	4.65563	1.87233	-3.29238
H	4.98519	2.56041	-2.5192
C	4.9419	2.15931	-4.62878
H	5.4896	3.06789	-4.85061
C	4.54863	1.30044	-5.66421
C	3.83854	0.14505	-5.29425
H	3.51287	-0.5552	-6.05794
C	3.54508	-0.14276	-3.96499
H	3.00303	-1.05063	-3.71799
C	5.77057	0.41889	-7.67801
H	6.01407	0.58473	-8.73353
H	5.27483	-0.55306	-7.59876
H	6.70925	0.36162	-7.11746
C	4.87685	1.56427	-7.14485
C	5.62673	2.89429	-7.34881
H	5.83118	3.0424	-8.41401
H	6.58782	2.9053	-6.82474
H	5.03839	3.75078	-7.00364

C	3.56857	1.6165	-7.96865
H	2.91661	2.42356	-7.61966
H	3.00629	0.6807	-7.90133
H	3.79324	1.79374	-9.0264
C	3.1586	-1.01272	2.59443
C	2.25882	-0.28803	3.39332
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C	2.09834	-0.58132	4.74308
H	1.39473	0.01174	5.31993
C	2.82401	-1.60975	5.36975
C	3.72066	-2.32947	4.56861
H	4.30844	-3.13446	4.99414
C	3.88677	-2.03788	3.21291
H	4.5876	-2.62485	2.62663
C	2.62171	-1.89568	6.86854
C	1.14017	-2.25631	7.13004
H	0.85081	-3.15328	6.57274
H	0.46536	-1.44765	6.83479
H	0.97787	-2.45222	8.19595
C	2.99289	-0.63508	7.68574
H	2.84851	-0.81908	8.75632
H	2.37618	0.22523	7.40971
H	4.04043	-0.35993	7.5261
C	3.49477	-3.06385	7.36378
H	3.26553	-3.99551	6.83633
H	3.31194	-3.23455	8.42951
H	4.56262	-2.85527	7.24208
C	1.17355	0.6858	-1.57824
C	-0.08992	0.19584	-1.15265
C	-1.28839	0.80458	-1.595
C	-1.19948	1.86623	-2.51056
H	-2.11072	2.28538	-2.90416
C	0.02575	2.38295	-2.9319
C	1.19414	1.79283	-2.43594
H	2.14631	2.2134	-2.72039
C	0.13253	3.58011	-3.89733

C	0.82752	4.75633	-3.17068
H	0.24728	5.07281	-2.29765
H	0.92611	5.6154	-3.84435
H	1.83057	4.48677	-2.8271
C	-1.24374	4.06618	-4.3873
H	-1.78132	3.28347	-4.93302
H	-1.11024	4.91063	-5.07176
H	-1.87866	4.40358	-3.56324
C	0.96643	3.17944	-5.13637
H	0.49666	2.34622	-5.66916
H	1.98117	2.87496	-4.86934
H	1.042	4.02592	-5.82909
C	-7.49416	0.13958	-1.33584
C	7.05419	0.01735	1.11785
H	6.35342	0.3724	-2.18936
C	8.88933	1.76734	2.37099
C	9.98698	1.96377	3.41829
H	9.24269	2.04906	1.37567
H	8.00645	2.36546	2.61654
C	10.44425	3.4264	3.51394
H	9.6231	1.62906	4.39835
H	10.84617	1.32721	3.17049
H	10.81489	3.7569	2.53379
H	9.57875	4.06373	3.74325
C	9.56962	-1.34597	-0.87808
C	10.96042	-1.42294	-1.51056
H	9.60906	-1.60629	0.18281
H	8.87542	-2.02415	-1.3837
C	11.55339	-2.83623	-1.42078
H	10.90527	-1.11335	-2.56228
H	11.62961	-0.71145	-1.00985
H	11.60921	-3.13916	-0.36604
H	10.8704	-3.5476	-1.90588
C	12.94354	-2.95696	-2.05812
C	13.53284	-4.36949	-1.96313
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H	12.88648	-2.65681	-3.11402
C	14.91799	-4.50467	-2.60767
H	13.59399	-4.66558	-0.90618
H	12.84259	-5.0823	-2.4365
C	15.50374	-5.91815	-2.50709
H	14.85633	-4.21198	-3.66561
H	15.60895	-3.79093	-2.13671
H	15.56821	-6.20993	-1.44893
H	14.81108	-6.63257	-2.97488
C	16.88675	-6.05978	-3.15482
C	17.46266	-7.47489	-3.04785
H	17.57936	-5.34631	-2.6879
H	16.82192	-5.76994	-4.21244
H	18.44996	-7.543	-3.51621
H	17.56945	-7.78088	-2.00085
H	16.81073	-8.20629	-3.53907
C	11.53217	3.65059	4.57178
C	11.99212	5.10991	4.6754
H	12.3973	3.01188	4.34417
H	11.15914	3.31714	5.55056
C	13.06936	5.3385	5.74281
H	12.37263	5.441	3.69862
H	11.12447	5.74878	4.89367
C	13.52875	6.7977	5.84848
H	12.68767	5.00694	6.71909
H	13.93727	4.69961	5.5255
H	13.91544	7.12889	4.87392
H	12.66025	7.43758	6.06127
C	14.60011	7.02877	6.92128
C	15.05295	8.48859	7.01952
H	15.46793	6.38955	6.70912
H	14.21302	6.69904	7.89507
H	15.81557	8.62135	7.79387
H	15.47845	8.83606	6.07115
H	14.21264	9.14838	7.26405
S	8.89754	0.3699	-1.02366

S	8.38216	-0.00951	2.32486
S	-9.09653	0.91468	-1.3357
S	-8.90876	-2.23965	-1.82709
C	-9.78839	-1.5308	-3.20266
C	-11.12993	-2.1972	-3.36904
H	-9.1681	-1.65985	-4.12246
H	-9.91282	-0.43668	-3.01601
H	-10.98333	-3.29839	-3.529
H	-11.72615	-2.07868	-2.42556
C	-11.9189	-1.60698	-4.55258
C	-13.28702	-2.23349	-4.63762
H	-11.34139	-1.79416	-5.49008
H	-12.00005	-0.5026	-4.40701
H	-13.18286	-3.34459	-4.75714
H	-13.83986	-2.05668	-3.67701
C	-14.10436	-1.66507	-5.81255
C	-15.47897	-2.28228	-5.84454
H	-13.55472	-1.87909	-6.76099
H	-14.17317	-0.55693	-5.69122
H	-15.38649	-3.39671	-5.94031
H	-16.00337	-2.07828	-4.87343
C	-16.32459	-1.73522	-7.00954
C	-17.69777	-2.35635	-6.99999
H	-15.79615	-1.96332	-7.96671
H	-16.39383	-0.62542	-6.90473
C	-18.55274	-1.84178	-8.12945
H	-17.60426	-3.47196	-7.07969
H	-18.20044	-2.13783	-6.02058
H	-19.56321	-2.31603	-8.10087
H	-18.68014	-0.73474	-8.05374
H	-18.0823	-2.0726	-9.11581
C	-10.29942	-0.20766	-0.65613
C	-11.44473	0.55654	-0.04314
H	-9.79496	-0.84333	0.11128
H	-10.66405	-0.87296	-1.4758
H	-11.05351	1.23722	0.75893

H	-11.92031	1.2078	-0.82374
C	-12.50567	-0.38564	0.55544
C	-13.63647	0.40932	1.15612
H	-12.01536	-1.02114	1.3321
H	-12.88218	-1.05422	-0.25615
H	-13.23305	1.09252	1.94996
H	-14.09758	1.05966	0.36612
C	-14.7171	-0.50348	1.76492
C	-15.84719	0.3209	2.32598
H	-14.24577	-1.1223	2.56639
H	-15.08947	-1.19041	0.96685
H	-15.44748	1.02164	3.10629
H	-16.28896	0.95385	1.51119
C	-16.9473	-0.56202	2.94387
C	-18.07981	0.29011	3.45651
H	-16.4966	-1.15833	3.77377
H	-17.31128	-1.27146	2.16179
C	-19.1754	-0.5443	4.06879
H	-17.68804	1.01253	4.22091
H	-18.50058	0.89984	2.61339
H	-20.00134	0.10871	4.44051
H	-19.59754	-1.25321	3.31596
H	-18.78272	-1.14021	4.92797

E(SCF)=-6106.29033918 a.u.

E(zp)=-6103.871624 a.u.