Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Scanning Tunneling Microscopy Analysis of Octameric *o*-Phenylenes on Au(111)

Santiago Marqués-González,[a] Shintaro Fujii,[a†] Tomoaki Nishino,[a] Yoshiaki Shoji,[b] Fumitaka Ishiwari,[b] Takanori Fukushima,[b†] and Manabu Kiguchi[a†]

E-mail: fujii.s.af@m.titech.ac.jp; fukushima@res.titech.ac.jp; kiguti@chem.titech.ac.jp

[1] Department of Chemistry, Graduate School of Science and Engineering, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo 152-8551, Japan

[2] Chemical Resources Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

Table of contents

1. STM image on clean Au(111)

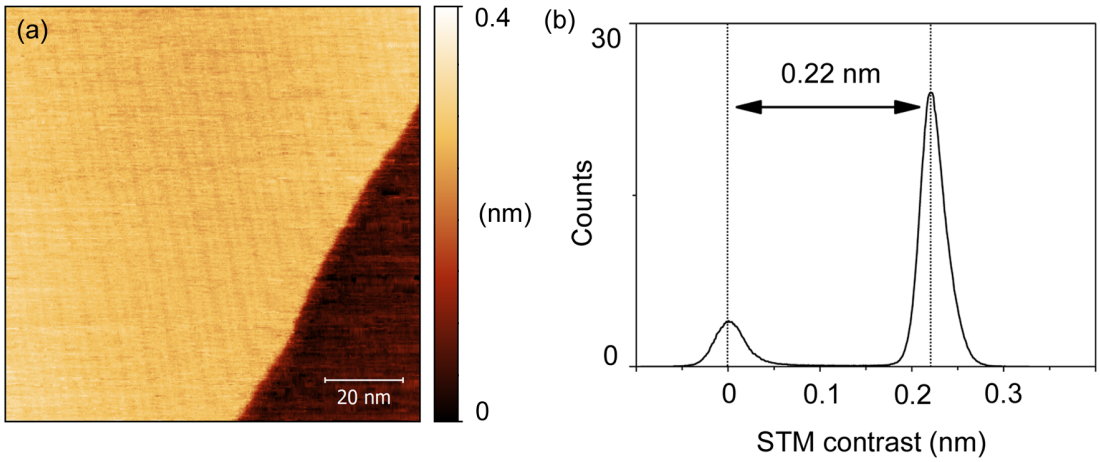

Figure S1. (a) STM image and (b) STM contrast (apparent height) distribution of the flame-annealed Au(111) substrate. Imaging area = 100 × 100 nm; tunneling current (I_t) = 200 pA; sample bias voltage (V_s) = 100 mV.

2. STM images of the OP_8Br and OP_8NO_2 films on Au(111)

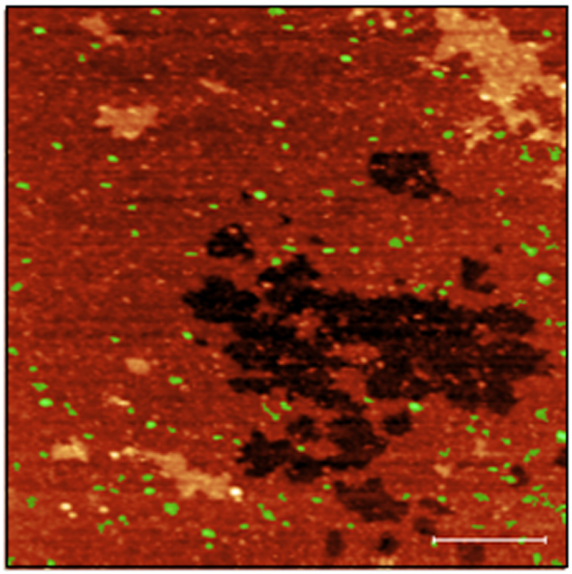

Figure S2. STM image of the OP_8Br film on Au(111) at the same area as that shown in Figure 2a. The bright spots are highlighted in green color for clarity.

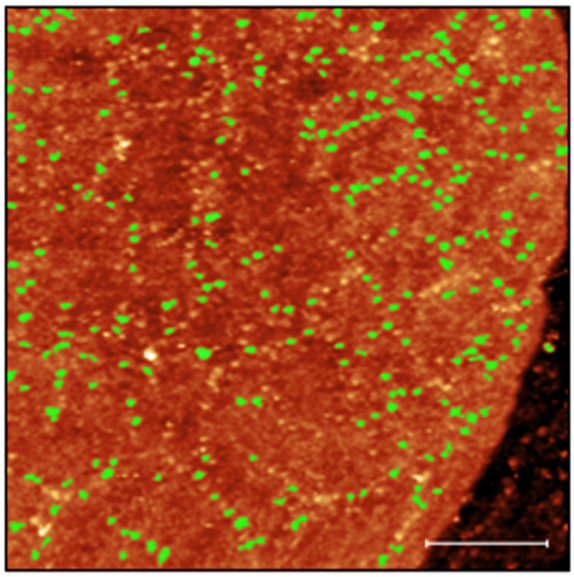

Figure S3. STM image of the OP_8NO_2 film on Au(111) at the same area as that shown in Figure 5a. The bright spots are highlighted in green color for clarity.

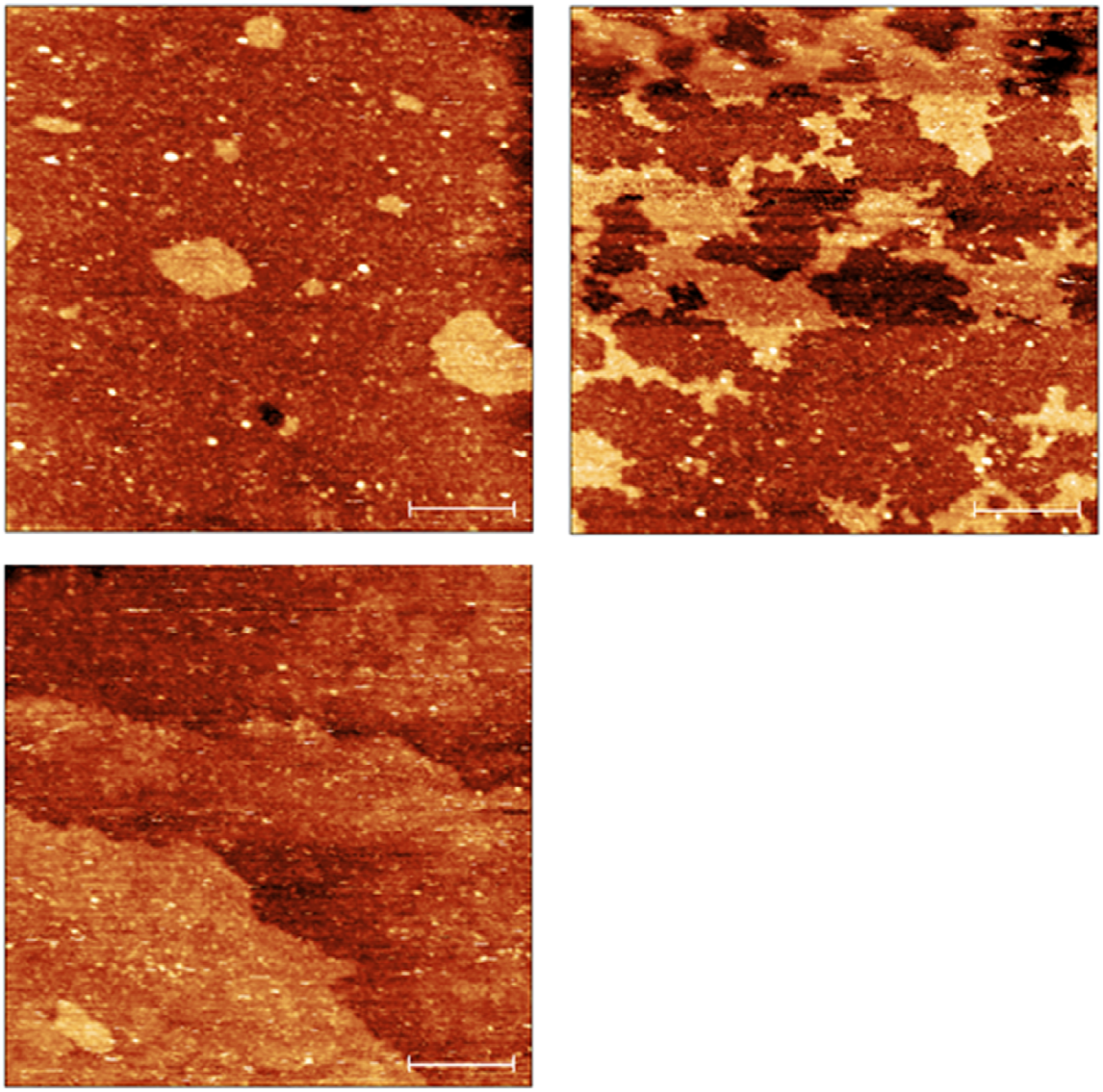

Figure S4. Series of STM images corresponding to OP_8Br films obtained by three different sets of Au-tip and sample. Film morphology was found to be consistent among samples and different electro-etched Au tips. Scale bar = 20 nm; I_t = 20 pA; V_s = 1.5 V.

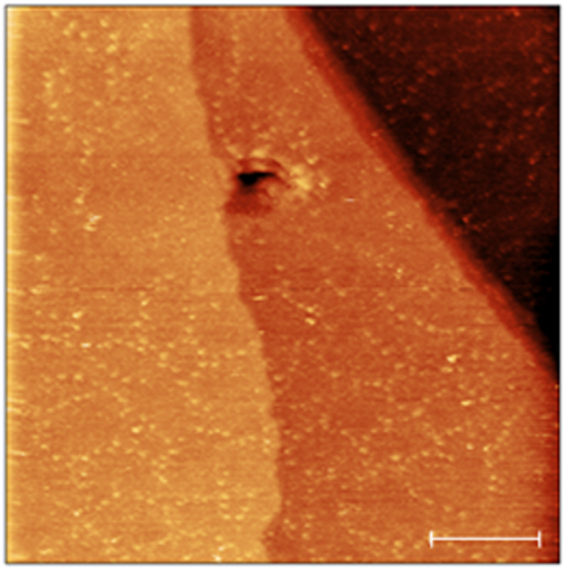

Figure S5. STM image corresponding to OP_8NO_2 film obtained by the same set of the Au tip and the sample as presented in Figure 5. Film morphology was consistent among samples and different electro-etched Au tips. Scale bar = 20 nm. Scale bar = 20 nm; I_t = 20 pA; V_s = 1.5 V.

3. Bias dependence of the STM contrast for the molecular films on Au(111)

To check bias voltage dependence of STM contrast (apparent height) on the molecular film, we analyzed STM contrast distribution (apparent height distribution) of the molecular films. Figure S6 shows STM images of the OP_8Br film on Au(111) recorded at different bias voltages of +1.5, +1.0 and -1.0 V, and corresponding STM contrast-histograms. The STM contrast distribution on the molecular film is described by two Gaussian peaks, which can be ascribed to the coexistence of different OP8Br-conformers as discussed in the main text. The peak separation of the two Gaussian peaks are 0.06, 0.045, 0.03 nm at the bias voltages of +1.5, +1.0 and -1.0 V, respectively (Figure S7). At the positive sample bias voltage, we found a weak bias voltage-dependence of the STM contrast for the molecular films. At the negative sample bias voltage, relative STM contrast is qualitatively similar as observed at the positive sample bias voltage. At the sample bias voltage of +1.0–1.5 V used for the molecular imaging (see Figures 2,3,5,6), lowest unoccupied molecular orbitals (LUMOs) contribute STM contrast. Figure S8 shows calculated molecular orbital energies of the perfectly and partially folded conformers for OP8Br, in which the LUMO lies far from the Fermi energy of Au (-5.1 eV)[s1] for both conformers (perfectly folded conformer; -0.2 eV, partially folded conformer; -0.6 eV). The energy mismatch causes small but finite local density of states (so-called the tail of the LUMO density of states) within the tunneling voltages for the weakly coupled molecular system on the Au surface and is responsible for the observed weak voltage-dependence of the STM contrast (Figure S7).

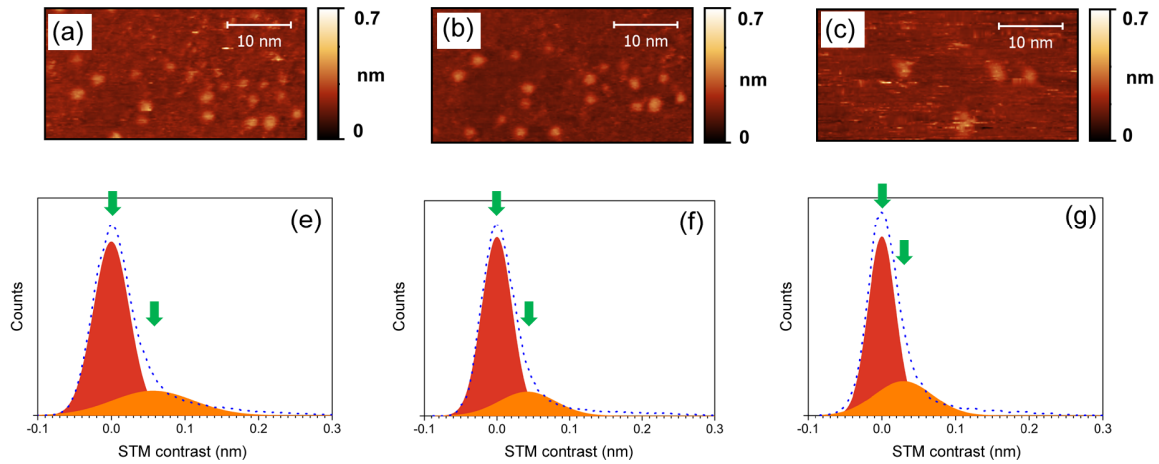

Figure S6. (a-c) STM images of the OP_8Br film on Au(111) recorded at difference sample bias voltages of (a) +1.5 V, (b) +1.0 V and (c) -1.0V. Imaging area = 40 × 20 nm; tunneling current (I_t) = 200 pA. (d-f) Histograms of the STM contrast in (a), (b) and (c) are in (d), (e) and (f), respectively. The dotted curve and filled peaks indicate raw counts and separated Gaussian distributions, respectively.

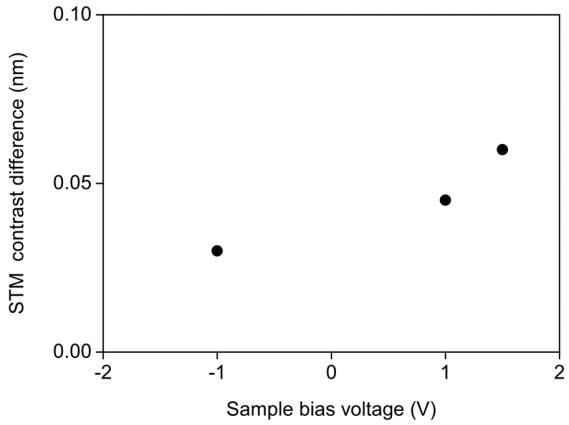

Figure S7. Bias voltage-dependence of the STM contrast-difference (the peak-separation in the histograms in Figure S6. See arrows in Figure S6).

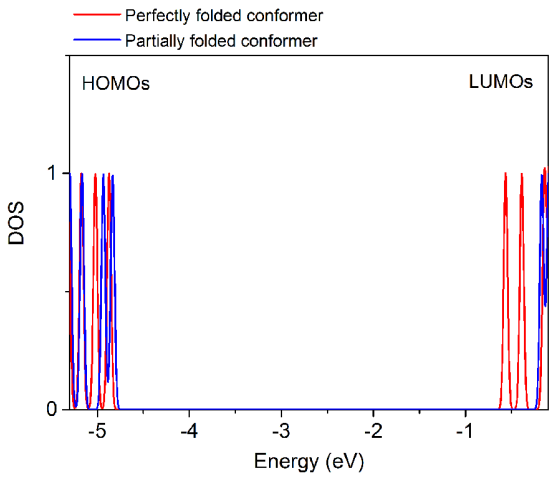

Figure S8. Calculated energy levels of the molecular orbitals for the perfectly and partially folded conformers for OP_8Br. The LUMO is indicated by an arrow (perfectly folded conformer; -0.2 eV, partially folded conformer; -0.6 eV).

4. Molecular scale STM contrast for the molecular films on Au(111)

During repeated STM imaging on the molecular film for OP_8Br, a small fraction of STM images featured molecular scale contrast (Figure S9), in which nanometer-sized brighter protrusions randomly distribute over the Au(111) substrate. Such almost regularly shaped protrusions could not be explained by pollution and are from the adsorbed molecules on the Au(111).

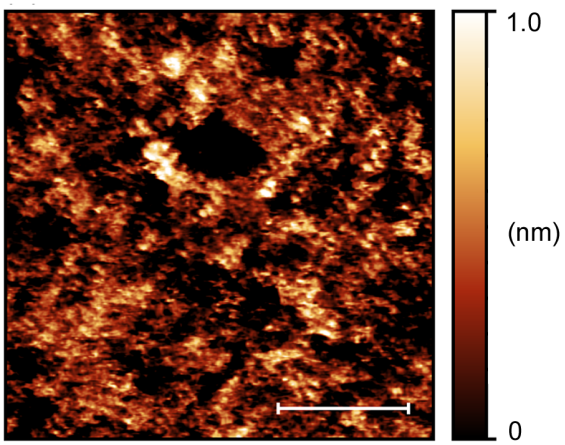

Figure S9. STM images of the molecular film for OP_8Br. Imaging area = 33 × 33 nm; I_t = 200 pA; V_s = 1.5 V. Scale bar = 10 nm.

5. Appendix. Cartesian coordinates (in Å) and energies of the optimized structures

Perfectly folded OP_8Br conformer			
Energy = -8824.13720115 A.U.			
	X	Y	Z
O	-7.156233	-3.31823	-0.106132
O	-5.490477	-3.256968	-2.098364
O	-2.147466	4.94415	-1.958931
O	-3.952498	3.978381	-3.5556
O	-0.788492	-3.604862	-3.103309
O	-2.312952	-4.354772	-1.136885
O	2.313041	4.354568	-1.136797
O	0.788546	3.604724	-3.103258
O	3.952642	-3.977932	-3.555847
O	2.147618	-4.943964	-1.959361
O	7.156194	3.318355	-0.105922
O	5.490568	3.257117	-2.098251
C	-4.794243	0.111277	-0.65296
C	-5.765252	0.077752	0.34691
C	-6.564414	-1.049154	0.571806
H	-7.294145	-1.024637	1.370063
C	-6.438242	-2.168085	-0.244517
C	-5.514155	-2.140622	-1.318757
C	-4.706142	-1.021657	-1.489671
H	-3.962188	-1.011626	-2.276939
C	-3.956045	1.311809	-0.951093
C	-2.910625	1.778612	-0.135671
C	-2.306341	3.009208	-0.466683
H	-1.504071	3.369449	0.166534
C	-2.678687	3.746424	-1.586146
C	-3.67619	3.230049	-2.445781
C	-4.299043	2.034587	-2.111592
H	-5.104931	1.653896	-2.72833
C	-2.478696	1.118034	1.141749
C	-1.782552	-0.100631	1.254277
C	-1.532369	-0.615156	2.54516
H	-0.988564	-1.548928	2.622511
C	-1.915946	0.048348	3.704494
C	-2.56299	1.299069	3.588751
C	-2.822333	1.807118	2.323399
H	-3.357683	2.742071	2.220185
C	-1.364061	-0.961516	0.100814
C	-0.41195	-0.625257	-0.881898
C	-0.231623	-1.503218	-1.972085
H	0.49973	-1.233928	-2.724838
C	-0.899734	-2.717783	-2.070747
C	-1.755985	-3.111018	-1.017705
C	-1.9871	-2.225541	0.02612
H	-2.708389	-2.481382	0.792744
C	0.411908	0.625117	-0.881851
C	1.363966	0.961389	0.100911
C	1.987024	2.225399	0.026228
H	2.708258	2.481254	0.792902
C	1.755965	3.110869	-1.017614
C	0.89972	2.717656	-2.070664
C	0.23161	1.503091	-1.972035
H	-0.499725	1.233808	-2.724806
C	1.782431	0.100488	1.254373
C	2.478596	-1.118158	1.141754
C	2.822222	-1.807334	2.323356
H	3.357587	-2.742267	2.220076
C	2.562889	-1.299356	3.588735
C	1.91588	-0.048617	3.704565
C	1.532296	0.614971	2.545282
H	0.988512	1.54875	2.62269
C	2.910529	-1.778598	-0.135728
C	3.955952	-1.311639	-0.951057
C	4.299038	-2.03427	-2.111629
H	5.104936	-1.653474	-2.728287
C	3.67625	-3.229719	-2.445966
C	2.678718	-3.746237	-1.586438
C	2.306298	-3.009176	-0.466898
H	1.504039	-3.369538	0.166262
C	4.794068	-0.111067	-0.652804

C	5.765112	-0.077601	0.347044
C	6.564274	1.049297	0.571981
H	7.294024	1.02474	1.370221
C	6.438122	2.168259	-0.2443
C	5.514029	2.140849	-1.318536
C	4.705986	1.021904	-1.489472
H	3.962031	1.011906	-2.276743
C	-8.120366	-3.377169	0.932486
H	-7.658292	-3.25299	1.921074
H	-8.569889	-4.369525	0.865288
H	-8.900524	-2.615317	0.802487
C	-4.72708	-3.228305	-3.299569
H	-5.000365	-2.36519	-3.920766
H	-4.980965	-4.149481	-3.827599
H	-3.651472	-3.219688	-3.098213
C	-1.258985	5.600531	-1.063971
H	-1.70616	5.705114	-0.066518
H	-0.298078	5.081531	-0.989529
C	-4.996755	3.53862	-4.406088
H	-4.781729	2.551685	-4.838635
H	-5.059639	4.276955	-5.207958
H	-5.958057	3.494282	-3.87695
C	0.044174	-3.260422	-4.202087
H	-0.261589	-2.305634	-4.650996
H	-0.086656	-4.062017	-4.931551
H	1.098727	-3.212143	-3.911298
C	-3.138758	-4.825995	-0.079546
H	-2.60639	-4.809944	0.880779
H	-3.387493	-5.856812	-0.339164
H	-4.06403	-4.245771	0.001268
C	3.138963	4.825616	-0.079471
H	2.60666	4.809536	0.880889
H	4.064159	4.245246	0.001237
C	-0.044007	3.260238	-4.202114
H	0.261808	2.305448	-4.650974
H	0.086894	4.061815	-4.931587
H	-1.09859	3.211964	-3.91142
C	4.996882	-3.538003	-4.406268
H	4.781818	-2.551012	-4.838665
H	5.059797	-4.276217	-5.208247
H	5.958183	-3.493708	-3.877123

C	1.259125	-5.60049	-1.064521
H	1.706331	-5.705337	-0.067107
H	1.093155	-6.591195	-1.492567
H	0.298262	-5.081437	-0.989913
C	4.727265	3.228464	-3.299518
H	5.000537	2.365307	-3.920663
H	4.981305	4.149586	-3.827572
H	3.651647	3.21997	-3.09825
O	-1.705966	-0.392858	4.977219
O	-2.894106	1.915877	4.762857
O	2.894012	-1.91622	4.762812
O	1.706036	0.392548	4.977324
H	-1.093101	6.591353	-1.491788
H	3.387813	5.856418	-0.339029
C	-3.733405	3.056934	4.687105
C	3.733219	-3.057341	4.687002
C	-1.137656	-1.681996	5.160829
C	8.12037	3.377214	0.932659
C	1.137843	1.681721	5.161034
H	-1.163862	-1.862846	6.237227
H	-1.726931	-2.454354	4.648279
H	-0.097943	-1.721411	4.818802
H	-3.963456	3.328011	5.719598
H	-4.662419	2.830587	4.148253
H	-3.231298	3.902532	4.196648
H	7.658323	3.253067	1.921265
H	8.900466	2.615305	0.802628
H	8.569969	4.369536	0.86545
H	1.164144	1.862515	6.237439
H	1.727152	2.454057	4.648486
H	0.09811	1.721254	4.819091
H	3.963287	-3.328459	5.71948
H	4.66223	-2.831052	4.148119
H	3.231034	-3.902891	4.196543
Br	6.15402	-1.628292	1.408491
Br	-6.15402	1.628384	1.408503

Partially folded OP_8Br conformer			
Energy = -8824.12992959 A.U.			
	X	Y	Z
H	-0.931394	-1.754112	-1.192908
C	-1.910313	-1.311626	-1.339254
C	-4.404361	-0.240224	-1.782055
C	-2.452282	-0.469451	-0.352995
C	-2.570563	-1.625109	-2.516916
C	-3.845583	-1.071737	-2.750311
C	-3.750624	0.059111	-0.56833
H	-5.376475	0.198125	-1.960886
C	-1.618413	-0.19458	0.862374
C	-0.149834	0.223861	3.246168
C	-2.154382	-0.519437	2.124652
C	-0.313171	0.338327	0.796119
C	0.387196	0.542351	2.00558
C	-1.456005	-0.320028	3.307356
H	-3.149633	-0.940189	2.153052
H	1.38929	0.947275	1.956232
C	0.35272	0.743154	-0.48609
C	1.480882	1.630464	-2.923477
C	1.658934	0.333986	-0.849552
C	-0.349124	1.606337	-1.351807
C	0.181253	2.044486	-2.562626
C	2.184716	0.795504	-2.069232
H	-1.348057	1.912435	-1.070878
H	3.175358	0.48482	-2.378128
C	2.481932	-0.59563	-0.009117
C	3.842278	-2.477451	1.620569
C	1.927097	-1.848017	0.305646
C	3.775684	-0.296062	0.487202
C	4.413126	-1.243903	1.314986
C	2.571232	-2.786287	1.096193
H	0.950661	-2.118186	-0.080389
H	5.382016	-0.994342	1.724864
C	4.484724	0.99961	0.232742
C	5.709767	3.539457	-0.152104
C	5.852518	1.089179	-0.102413
C	3.766826	2.206031	0.381359
C	4.340285	3.455993	0.191743
C	6.434628	2.361757	-0.282512
H	2.720357	2.149211	0.645664
H	7.48322	2.403769	-0.55286
C	6.791238	-0.071803	-0.219479
C	8.701673	-2.180694	-0.308456
C	6.768662	-1.03767	-1.221801
C	7.832017	-0.174461	0.73323
C	8.77575	-1.195338	0.708986
C	7.698322	-2.084645	-1.266723
H	7.870936	0.577081	1.51331
O	-4.444275	-1.403135	-3.933169
O	0.484576	0.392236	4.441617
O	-0.471022	2.853966	-3.450203
O	4.424099	-3.433731	2.404306
O	3.684421	4.64459	0.316295
O	9.649748	-3.154452	-0.265716
C	9.60957	-4.165217	-1.261826
H	8.665397	-4.724588	-1.229665
H	10.438025	-4.838273	-1.034784
H	9.746491	-3.745711	-2.267244
C	2.295266	4.610229	0.600581
H	1.971113	5.652732	0.61721
H	2.093242	4.153834	1.579571
H	1.73651	4.063518	-0.170115
C	5.734234	-3.193977	2.892593
H	6.445168	-3.02603	2.074027
H	6.01689	-4.094294	3.441702
H	5.761499	-2.332335	3.573919
C	-1.821105	3.194791	-3.173951
H	-2.449627	2.300853	-3.073359
H	-2.159067	3.785927	-4.027414
H	-1.908995	3.798341	-2.260145
C	1.818375	0.872344	4.421922
H	2.479657	0.210995	3.846793
H	2.14125	0.895286	5.464683
H	1.878596	1.887044	4.003968
C	-5.756431	-0.922984	-4.1774
H	-5.782226	0.174023	-4.234819
H	-6.45899	-1.257657	-3.40396
H	-6.05142	-1.339832	-5.142359

C	-4.448599	0.971543	0.394713
C	-5.652759	2.829393	2.183843
C	-3.724606	2.045322	0.957026
C	-5.811419	0.850072	0.740005
C	-6.383162	1.78799	1.626431
C	-4.287561	2.96007	1.836459
H	-2.680835	2.149253	0.696446
H	-7.428612	1.667306	1.885068
C	-6.759857	-0.164563	0.180497
C	-8.694604	-1.932436	-0.935023
C	-6.744943	-1.530398	0.44663
C	-7.807841	0.303282	-0.646934
C	-8.762891	-0.540959	-1.202132
C	-7.685273	-2.409638	-0.105742
H	-7.843068	1.36645	-0.854221
O	-3.627137	4.005003	2.407897
O	-9.653423	-2.698816	-1.518864
C	-2.234248	4.12489	2.164931
H	-2.023426	4.313282	1.103005
H	-1.688915	3.227877	2.484812
H	-1.904801	4.983235	2.75369
C	-9.620695	-4.09872	-1.28494
H	-8.682401	-4.544382	-1.640371
H	-10.456424	-4.513381	-1.850986
H	-9.751251	-4.332345	-0.220058
O	-9.788439	-0.145602	-2.006111
C	-9.917721	1.237457	-2.290019
H	-9.039631	1.625674	-2.823802
H	-10.797649	1.328603	-2.929191
H	-10.070004	1.825645	-1.375246
O	-6.140257	3.757144	3.054791
C	-7.497891	3.651341	3.446132
H	-8.176779	3.755455	2.588591
H	-7.701198	2.696513	3.949439
H	-7.671653	4.472143	4.144478
O	-1.993645	-2.506251	-3.39794
C	-1.512552	-1.927287	-4.614157
H	-0.762253	-1.152912	-4.407757
H	-1.046475	-2.742442	-5.17266
H	-2.330385	-1.50019	-5.204125
O	-1.923701	-0.613857	4.552845
C	-3.239566	-1.134869	4.657281
H	-3.984719	-0.446465	4.239002
H	-3.331993	-2.104784	4.15016
H	-3.421441	-1.267197	5.725622
O	2.037656	1.978124	-4.131902
C	2.423147	3.34835	-4.254279
H	1.55679	4.015643	-4.193859
H	2.889686	3.445193	-5.237721
H	3.15214	3.619516	-3.47888
O	1.981234	-4.00926	1.305334
C	1.487421	-4.228454	2.628786
H	0.743463	-3.467164	2.898503
H	1.010724	-5.211587	2.614514
H	2.29883	-4.22601	3.364206
O	6.207624	4.795942	-0.329111
C	7.570654	4.92353	-0.694663
H	7.754449	5.995297	-0.79081
H	7.780764	4.431016	-1.653617
H	8.237355	4.509196	0.074033
O	9.795588	-1.344273	1.600037
C	9.930199	-0.374958	2.62541
H	10.803806	-0.675796	3.206426
H	10.095642	0.629519	2.213397
H	9.048825	-0.352457	3.280789
Br	-5.450984	-2.299818	1.627905
H	-7.619395	-3.462783	0.132909
Br	5.48624	-0.971261	-2.636245
H	7.629044	-2.809523	-2.066809

Perfectly folded OP_8NO_2 conformer			
Energy = -4090.93076564 A.U.			
	X	Y	Z
O	2.862212	7.240852	0.159648
O	2.011676	6.163336	-2.04061
O	5.05369	3.545162	2.705954
O	5.707718	2.178608	1.1439
O	4.802981	-2.164796	-2.057406
O	5.529156	-0.193252	-3.584225
O	-1.705994	3.226689	-3.198079
O	-1.108797	4.804717	-1.218865
O	1.108797	-4.804717	-1.218865
O	1.705994	-3.226689	-3.198079
O	-5.529156	0.193252	-3.584225
O	-4.802981	2.164796	-2.057406
O	-2.862212	-7.240852	0.159648
O	-2.011676	-6.163336	-2.04061
O	-5.05369	-3.545162	2.705954
O	-5.707718	-2.178608	1.1439
N	-5.019886	-3.116665	1.546393
N	5.019886	3.116665	1.546393
C	3.627151	3.162116	-0.545194
C	4.135783	3.795896	0.597547
C	3.883551	5.147754	0.877101
H	4.284171	5.557928	1.79329
C	3.163328	5.925348	-0.01355
C	2.684702	5.332492	-1.212746
C	2.90496	3.975029	-1.438543
H	2.474539	3.501236	-2.311963
C	3.806841	1.720996	-0.89419
C	3.317609	0.653969	-0.12161
C	3.65982	-0.656485	-0.504326
H	3.287857	-1.477635	0.097137
C	4.424543	-0.925437	-1.635902
C	4.83747	0.149115	-2.45641
C	4.529786	1.44795	-2.071165
H	4.894849	2.284637	-2.655247
C	2.555482	0.842195	1.157992
C	1.217595	1.267172	1.25793
C	0.677526	1.491184	2.542818
H	-0.357027	1.805792	2.611055
C	1.40908	1.289865	3.707451
C	2.741354	0.824936	3.604642
C	3.277722	0.595745	2.343933
H	4.310148	0.283275	2.250842
C	0.353856	1.624282	0.086326
C	-0.10488	0.741162	-0.911385
C	-0.784663	1.282105	-2.025009
H	-1.133606	0.596838	-2.788123
C	-1.074472	2.636128	-2.140633
C	-0.722657	3.49931	-1.078775
C	-0.007852	2.98568	-0.005162
H	0.337693	3.653906	0.774562
C	0.10488	-0.741162	-0.911385
C	-0.353856	-1.624282	0.086326
C	0.007852	-2.98568	-0.005162
H	-0.337693	-3.653906	0.774562
C	0.722657	-3.49931	-1.078775
C	1.074472	-2.636128	-2.140633
C	0.784663	-1.282105	-2.025009
H	1.133606	-0.596838	-2.788123
C	-1.217595	-1.267172	1.25793
C	-2.555482	-0.842195	1.157992
C	-3.277722	-0.595745	2.343933
H	-4.310148	-0.283275	2.250842
C	-2.741354	-0.824936	3.604642
C	-1.40908	-1.289865	3.707451
C	-0.677526	-1.491184	2.542818
H	0.357027	-1.805792	2.611055
C	-3.317609	-0.653969	-0.12161
C	-3.806841	-1.720996	-0.89419
C	-4.529786	-1.44795	-2.071165
H	-4.894849	-2.284637	-2.655247
C	-4.83747	-0.149115	-2.45641
C	-4.424543	0.925437	-1.635902
C	-3.65982	0.656485	-0.504326
H	-3.287857	1.477635	0.097137
C	-3.627151	-3.162116	-0.545194
C	-4.135783	-3.795896	0.597547
C	-3.883551	-5.147754	0.877101

H	-4.284171	-5.557928	1.79329
C	-3.163328	-5.925348	-0.01355
C	-2.684702	-5.332492	-1.212746
C	-2.90496	-3.975029	-1.438543
H	-2.474539	-3.501236	-2.311963
C	3.341114	7.878835	1.335413
H	2.936064	7.409852	2.241584
H	2.994384	8.911633	1.274205
H	4.437743	7.864169	1.381409
C	1.52941	5.658331	-3.284765
H	2.342413	5.214442	-3.872589
H	1.132778	6.526638	-3.813168
H	0.726051	4.930385	-3.136258
C	4.605458	-3.267688	-1.181673
H	5.025542	-3.06419	-0.188174
H	3.546955	-3.531566	-1.092228
C	6.030655	0.853931	-4.395814
H	5.222055	1.479813	-4.798441
H	6.554035	0.367618	-5.221392
H	6.734886	1.49129	-3.844533
C	-2.12398	2.404476	-4.279529
H	-1.278109	1.857887	-4.718206
H	-2.536529	3.087827	-5.024351
H	-2.903418	1.699481	-3.971786
C	-0.901701	5.688285	-0.124356
H	-1.35575	5.29673	0.795414
H	-1.393062	6.622294	-0.403774
H	0.162278	5.884759	0.046441
C	0.901701	-5.688285	-0.124356
H	1.35575	-5.29673	0.795414
H	-0.162278	-5.884759	0.046441
C	2.12398	-2.404476	-4.279529
H	1.278109	-1.857887	-4.718206
H	2.536529	-3.087827	-5.024351
H	2.903418	-1.699481	-3.971786
C	-6.030655	-0.853931	-4.395814
H	-5.222055	-1.479813	-4.798441
H	-6.554035	-0.367618	-5.221392
H	-6.734886	-1.49129	-3.844533
C	-4.605458	3.267688	-1.181673
H	-5.025542	3.06419	-0.188174
H	-5.140579	4.102928	-1.638051
H	-3.546955	3.531566	-1.092228
C	-1.52941	-5.658331	-3.284765
H	-2.342413	-5.214442	-3.872589
H	-1.132778	-6.526638	-3.813168
H	-0.726051	-4.930385	-3.136258
O	0.950664	1.491998	4.97444
O	3.407039	0.639072	4.779301
O	-3.407039	-0.639072	4.779301
O	-0.950664	-1.491998	4.97444
H	5.140579	-4.102928	-1.638051
H	1.393062	-6.622294	-0.403774
C	4.814206	0.438223	4.710546
C	-4.814206	-0.438223	4.710546
C	-0.353856	2.027578	5.145727
C	-3.341114	-7.878835	1.335413
C	0.353856	-2.027578	5.145727
H	-0.463717	2.192963	6.219238
H	-0.465167	2.98443	4.617784
H	-1.128253	1.328551	4.81189
H	5.163346	0.442282	5.745116
H	5.301695	1.24392	4.148828
H	5.062829	-0.528871	4.252134
H	-2.936064	-7.409852	2.241584
H	-4.437743	-7.864169	1.381409
H	-2.994384	-8.911633	1.274205
H	0.463717	-2.192963	6.219238
H	0.465167	-2.98443	4.617784
H	1.128253	-1.328551	4.81189
H	-5.163346	-0.442282	5.745116
H	-5.301695	-1.24392	4.148828
H	-5.062829	0.528871	4.252134

Partially folded OP_8NO_2 conformer			
Energy = -4090.91549084 A.U.			
	X	Y	Z
H	0.99777	-2.085775	0.860548
C	1.960836	-1.628178	1.057593
C	4.414242	-0.520795	1.61804
C	2.457759	-0.646207	0.182667
C	2.6427	-2.057693	2.184801
C	3.894868	-1.482391	2.481983
C	3.737651	-0.100263	0.451634
H	5.368832	-0.066912	1.847524
C	1.581148	-0.238116	-0.963471
C	-0.001262	0.431603	-3.207592
C	2.057281	-0.42733	-2.276855
C	0.281361	0.280968	-0.771928
C	-0.475134	0.617251	-1.915765
C	1.295935	-0.105884	-3.394588
H	3.046316	-0.847781	-2.408458
H	-1.47025	1.016981	-1.77654
C	-0.319483	0.526798	0.582402
C	-1.304362	1.050673	3.182257
C	-1.604508	0.066144	0.96117
C	0.425283	1.278236	1.514306
C	-0.039461	1.543799	2.800221
C	-2.058288	0.333155	2.265263
H	1.403945	1.634444	1.222573
H	-3.022379	-0.038788	2.595687
C	-2.484118	-0.720542	0.036653
C	-3.953897	-2.306601	-1.798939
C	-2.00043	-1.951789	-0.437639
C	-3.763007	-0.292525	-0.398902
C	-4.457373	-1.094995	-1.330407
C	-2.699593	-2.748035	-1.330904
H	-1.036825	-2.318286	-0.101067
H	-5.413986	-0.744939	-1.69428
C	-4.400226	0.997907	0.02332
C	-5.50544	3.529337	0.710869
C	-5.7527	1.110171	0.406168
C	-3.633032	2.181198	-0.008944
C	-4.147248	3.425945	0.330309
C	-6.27963	2.376283	0.731518
H	-2.59512	2.109794	-0.300965
H	-7.316963	2.431869	1.040057
C	-6.729252	-0.024642	0.433793
C	-8.645403	-2.136372	0.24817
C	-6.683258	-1.148274	1.265109
C	-7.803189	0.025297	-0.478069
C	-8.758171	-0.984726	-0.576998
C	-7.604314	-2.20061	1.160621
H	-7.858374	0.883216	-1.137127
O	4.511124	-1.927056	3.61785
O	-0.693721	0.728618	-4.345204
O	0.647763	2.251853	3.746226
O	-4.588189	-3.122316	-2.693505
O	-3.442029	4.591618	0.320663
O	-9.598794	-3.086626	0.0757
C	-9.509893	-4.264981	0.866493
H	-8.56693	-4.797074	0.687496
H	-10.347208	-4.892199	0.557053
H	-9.600183	-4.037474	1.936493
C	-2.057629	4.52786	0.016725
H	-1.686915	5.55031	0.112949
H	-1.884602	4.175776	-1.009738
H	-1.519355	3.873027	0.714001
C	-5.866568	-2.733273	-3.166378
H	-6.587951	-2.634621	-2.345209
H	-6.190529	-3.529095	-3.83991
H	-5.822485	-1.78573	-3.721154
C	1.9654	2.675895	3.435445
H	2.614137	1.826728	3.185291
H	2.339108	3.169155	4.335112
H	1.977002	3.391393	2.60146
C	-2.021115	1.204746	-4.207285
H	-2.657222	0.48645	-3.673174
H	-2.395761	1.339589	-5.224102
H	-2.054875	2.169098	-3.680724
C	5.787861	-1.402087	3.938304
H	5.747204	-0.318935	4.119481
H	6.518824	-1.605839	3.1453
H	6.09719	-1.90792	4.855023

C	4.394987	0.948203	-0.394965
C	5.541683	3.0594	-1.921264
C	3.640278	2.066164	-0.807596
C	5.754657	0.90779	-0.767471
C	6.302716	1.971728	-1.51218
C	4.174239	3.10306	-1.561684
H	2.595606	2.106556	-0.533483
H	7.346002	1.90885	-1.798261
C	6.716964	-0.169329	-0.372087
C	8.601546	-2.090412	0.593045
C	6.672871	-1.515125	-0.75338
C	7.774724	0.193636	0.485858
C	8.714034	-0.721159	0.958313
C	7.577657	-2.467644	-0.26072
H	7.82884	1.229232	0.799314
O	3.481111	4.193152	-1.99167
O	9.538379	-2.92319	1.112101
C	2.082661	4.22883	-1.751508
H	1.858186	4.273547	-0.676649
H	1.575008	3.359225	-2.187719
H	1.724297	5.141665	-2.23128
C	9.451619	-4.304161	0.783691
H	8.499607	-4.735964	1.117573
H	10.275886	-4.785607	1.311797
H	9.564854	-4.466613	-0.29589
O	9.751492	-0.417851	1.773532
C	9.940298	0.938894	2.154014
H	9.088222	1.315926	2.733963
H	10.835664	0.948114	2.777078
H	10.095969	1.581809	1.278604
O	6.001264	4.109766	-2.657373
C	7.353005	4.083739	-3.080659
H	8.045935	4.080968	-2.227799
H	7.561923	3.211753	-3.714887
H	7.50124	4.996415	-3.660849
O	2.110787	-3.061114	2.954585
C	1.593484	-2.648869	4.223905
H	0.804934	-1.895927	4.098305
H	1.168342	-3.545169	4.681226
H	2.385569	-2.250021	4.866562
O	1.686306	-0.273374	-4.686382
C	3.005651	-0.749499	-4.923617
H	3.757789	-0.070015	-4.506584
H	3.162406	-1.747038	-4.496351
H	3.109296	-0.794997	-6.00965
O	-1.77006	1.217997	4.464915
C	-2.25975	2.525727	4.761135
H	-1.465378	3.277335	4.685705
H	-2.627029	2.487556	5.789664
H	-3.086691	2.794894	4.090647
O	-2.180506	-3.96435	-1.699015
C	-1.691618	-4.039301	-3.041012
H	-0.907161	-3.290788	-3.212746
H	-1.267632	-5.040072	-3.151936
H	-2.498247	-3.90053	-3.768647
O	-5.944032	4.778931	1.032239
C	-7.287332	4.921957	1.459289
H	-7.418826	5.983091	1.679197
H	-7.488969	4.334951	2.365319
H	-7.996804	4.624965	0.674481
O	-9.812222	-0.977249	-1.427934
C	-10.001469	0.157882	-2.2619
H	-10.910534	-0.042649	-2.830718
H	-10.133921	1.072241	-1.6699
H	-9.160695	0.293345	-2.954431
H	7.457616	-3.492482	-0.582893
H	-7.480986	-3.047078	1.821578
N	5.712233	-2.009605	-1.738708
O	5.424533	-3.207276	-1.718925
O	5.274159	-1.208274	-2.56878
N	-5.695543	-1.276033	2.338369
O	-5.400698	-2.410479	2.718163
O	-5.244545	-0.239689	2.829835

6. Reference

[S1] Michaelson, H. B. The work function of the elements and its periodicity. *J. Appl. Phys.*, **1977**, *48*, 4729–4733.