ADVANCED MATERIALS

Supporting Information

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Thermoelectric Properties of Solution-Processed n-Doped Ladder-Type Conducting Polymers

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Cyclic voltammetry

A BioLogic SP200 potentiostat was used for the electrochemical measurements with the three electrode setup. 0.1 M tetrabutylammonium hexafluoroborate (TBAP) in dry acetonitrile was utilized as a supporting electrolyte. Platinum disk (diam. 1 mm) and platinum wire were used as reference electrode and counter electrode, respectively. An Ag/Ag^+ quasi-reference electrode (QRE) was used (0.01 M $AgNO_3$ in 0.1 M TBAP). After each experiment, the system was calibrated by measuring the ferrocene/ferrocenium (Fc/Fc^+) redox potential, which was +0.096 V with respect to QRE. All measurements were carried out in a glove box under dry nitrogen.

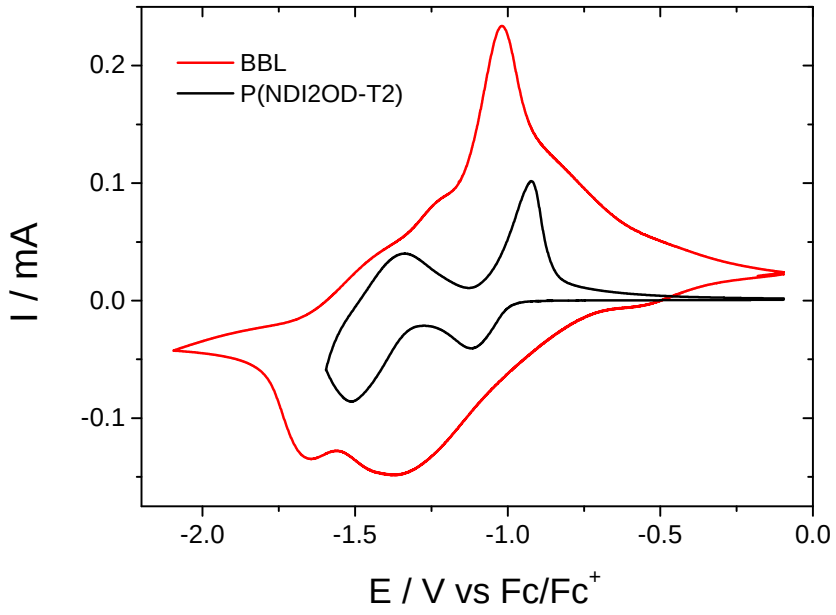


Figure S1. Cyclic voltammograms of P(NDI2OD-T2) and BBL (scan rate 20 mV/s).

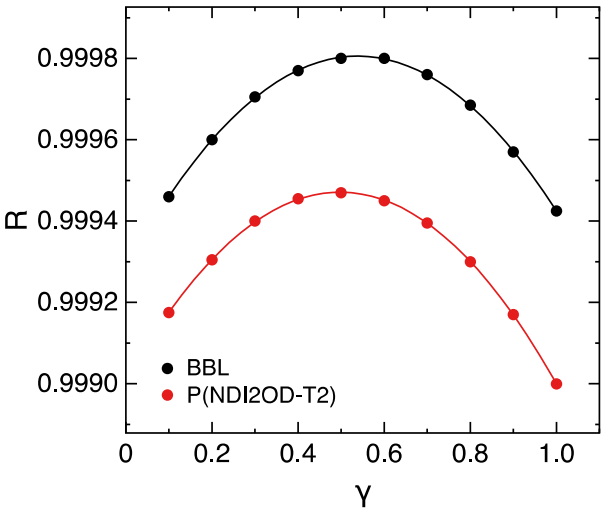


Figure S2. Evaluation of the Mott variable-range hopping exponent.

Structural charaterization

GIWAXS experimental: The silicon substrate surface was aligned at a grazing incident angle of 0.18° with respect to the incoming X-ray beam, supplied by a rotating Cu anode operated at 50 kV, 200 mA in point focus mode. The Cu k-alfa radiation (wavelength (λ) = 1.542 Å) was collimated and monochromatized with a 1D multilayer optic. The scattered radiation was recorded in vacuum on photo-stimulable imaging plates 121.5 mm from the sample. For further details of the instrumental setup, please refer to [Apitz, D., Bertram, R.P., Benter, N., Hieringer, W., Andreasen, J.W., Nielsen, M.M., Johansen, P.M., and Buse, K., 2005, Investigation of chromophore-chromophore interaction by electro-optic measurements, linear dichroism, x-ray scattering, and density-functional calculations: Physical Review E, v. 72, no. 3, p. 036610, 10 p.]. The data integration and conversion to reciprocal space coordinates was done with Matlab scripts described in [Breiby, D.W., Bunk, O., Andreasen, J.W., Lemke, H.T., and Nielsen, M.M., 2008, Simulating X-ray diffraction of textured films: Journal of Applied Crystallography, v. 41, no. Part 2, p. 262–271.]

TEM experimental: Electron microscopy was performed using the Linköping double corrected FEI Titan^3 G2 60-300. Images were recorded at low accelerating voltage (60 kV) to reduce knock on damage to the material and in monochromated TEM mode, with a beam limiting slit inserted in the first condenser image plane to reduce beam current to ~1 nA. The energy spread in monochromated mode was ¨150 mev (FWHM) which significantly reduces the impact of chromatic aberration (Cc) and extends the point resolution for lattice resolved imaging (<1.3Å). The samples were imaged in plan-view geometry.

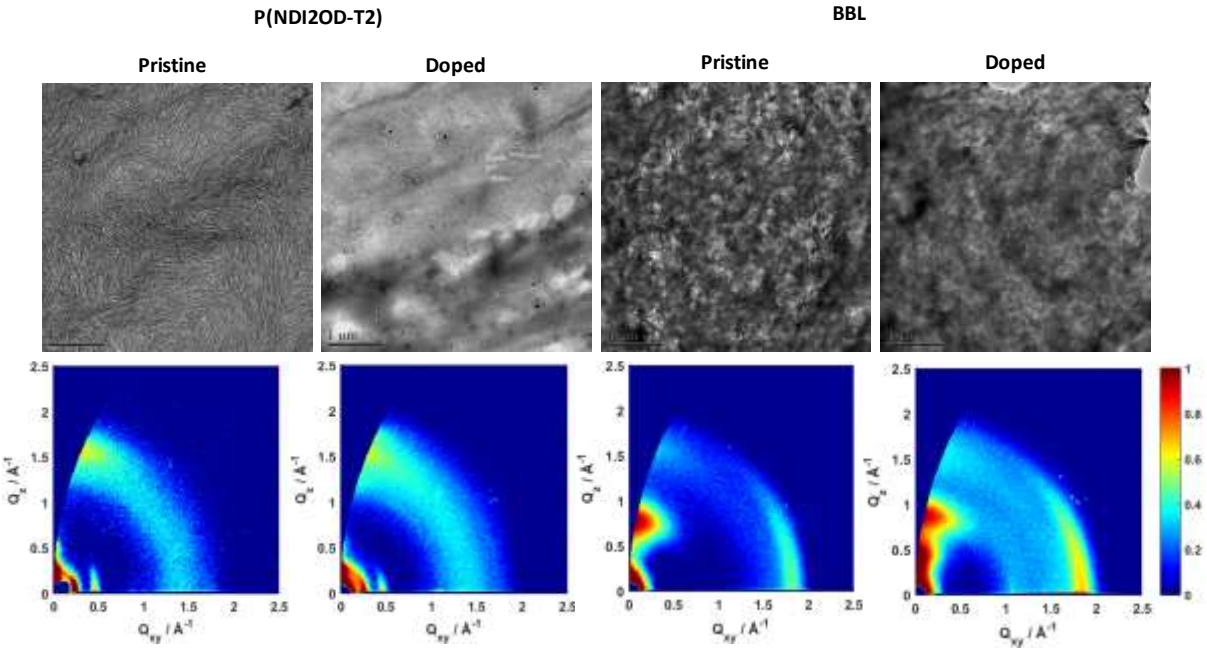


Figure S3. TEM images and GIWAXS patterns of pristine and doped P(NDI2OD-T2) and BBL.

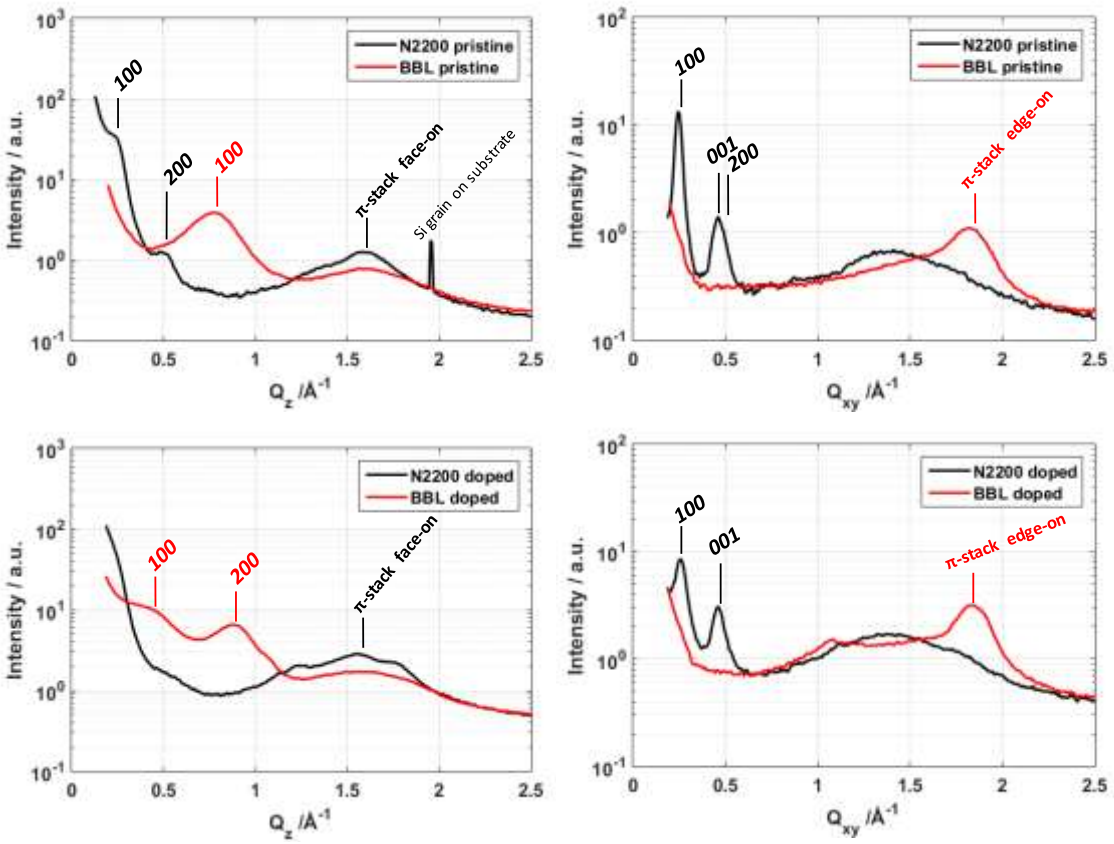


Figure S4. GIWAXS line cuts for pristine and doped P(NDI2OD-T2) [N2200] and BBL along the q_{xy} and q_z axes.

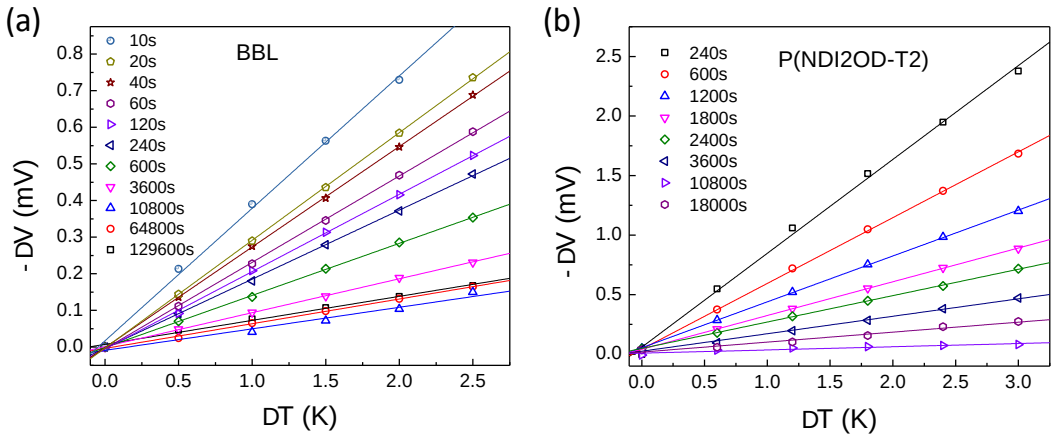


Figure S5. Thermal voltage as a function of ΔT for BBL (a) and P(NDI2OD-T2) (b) films for different TDAE doping time. The error bar in the final Seebeck coefficient values is obtained from the standard linear fitting error.

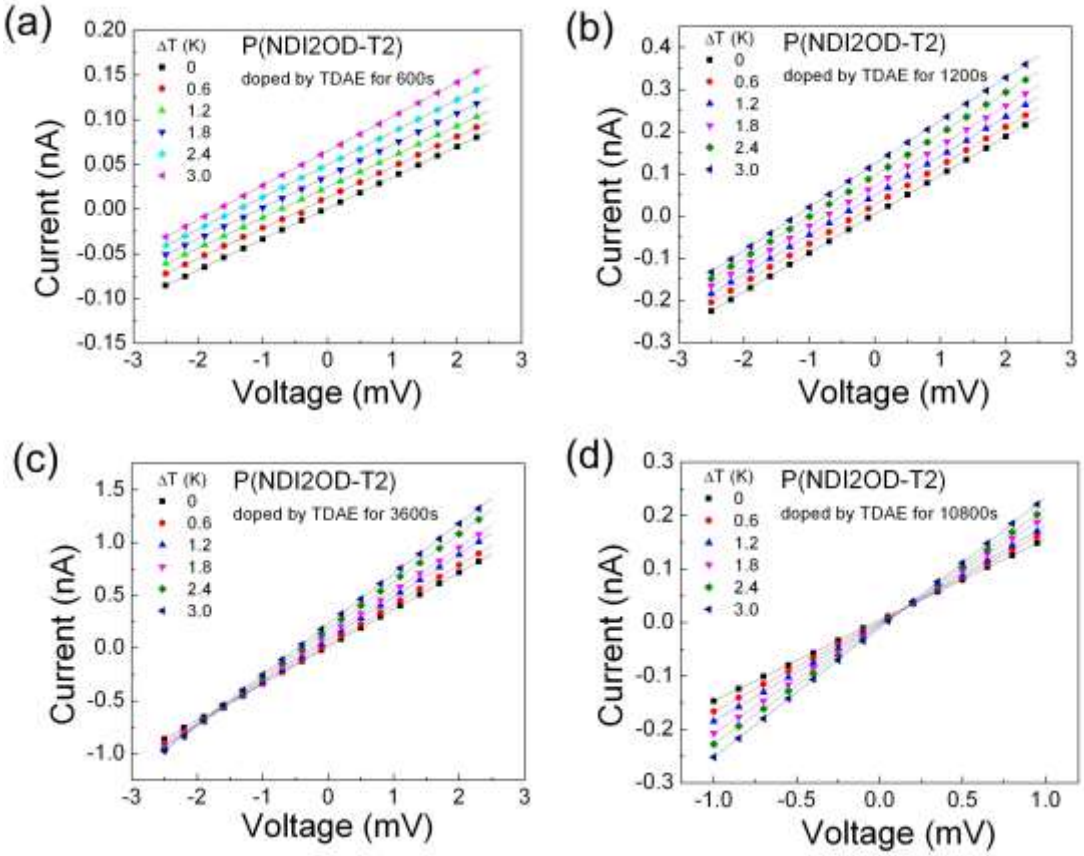


Figure S6. Current-voltage (I-V) curves for P(NDI2OD-T2) films doped by TDAE for different time. For (a) 600s, and (b) 1200s when the samples are not saturated, the slopes remain roughly same with increasing ΔT, whereas for (c) 3600s and (d) 10800s when the samples are saturated or oversaturated, the slopes changes with increasing ΔT.

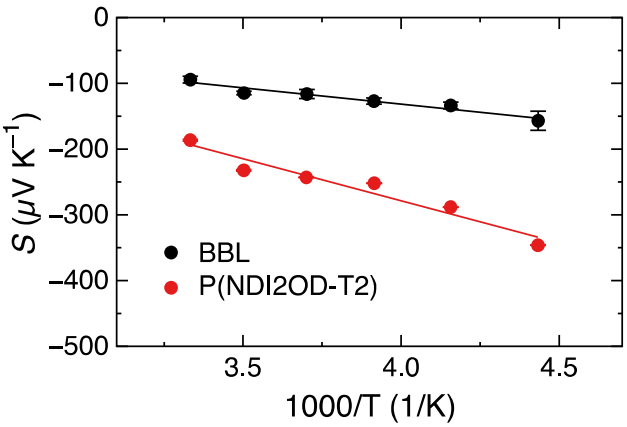


Figure S7. Temperature dependence of Seebeck coefficient for doped BBL and P(NDI2OD-T2) films.

Computational results

Computed TDDFT (ωB97X-D3/6-31G*) vertical excitation energies (eV) and oscillator strengths for the longest oligomers of BBL (n=8) and P(NDI2OD-T2) (n = 5) in their neutral and charged states, respectively.

BBL, n = 8 ωB97X-D/6-31G* *Neutral state*	Energy eV	Oscillator Strength
S1	**2.7701**	**9.1965**
S2	2.8335	0.5543
S3	2.8991	0.4547
S4	2.9525	0.0617
S5	2.9909	0.0847
S6	3.0157	0.0125
S7	3.0289	0.0162
S8	3.0358	0.0011
S9	3.5222	0.3993
S10	3.5340	0.0227

BBL, n = 8 UωB97X-D/6-31G* *Charged (-1) state*	Energy eV	Oscillator Strength
D1	*-0.1610*	*-0.0094*
D2	*-0.1188*	*-0.0016*
D3	*-0.0467*	*-0.0777*
D4	0. 2645	0.0032
D5	0.2647	0.0022
D6	0.3134	0.0000
D7	0.3137	0.0000
D8	1.5554	0.0362
D9	1.6578	0.0000
D10	1.6621	0.0057

BBL, n = 8 UωB97X-D/6-31G* **broken symmetry (BS)** *Charged (-1) state*	Energy eV	Oscillator Strength
D1	1.1460	0.0039
D2	1.1680	0.0094
D3	1.1922	0.0002
D4	1.2375	0.0000
D5	1.2439	0.0000
D6	1.2711	0.0001
D7	1.2878	0.0001
D8	1.5891	0.0001
D9	1.5901	0.0001
D10	1.6697	0.0000
D11	1.6749	0.0000
D12	1.6930	0.0000
D13	1.7113	0.0000
D14	1.7228	0.0000

D15	1.9209	0.0277
D16	2.1614	0.6552
D17	2.4079	0.4653
D18	2.4228	0.0035
D19	**2.4980**	**3.5809**
D20	2.5840	0.0380

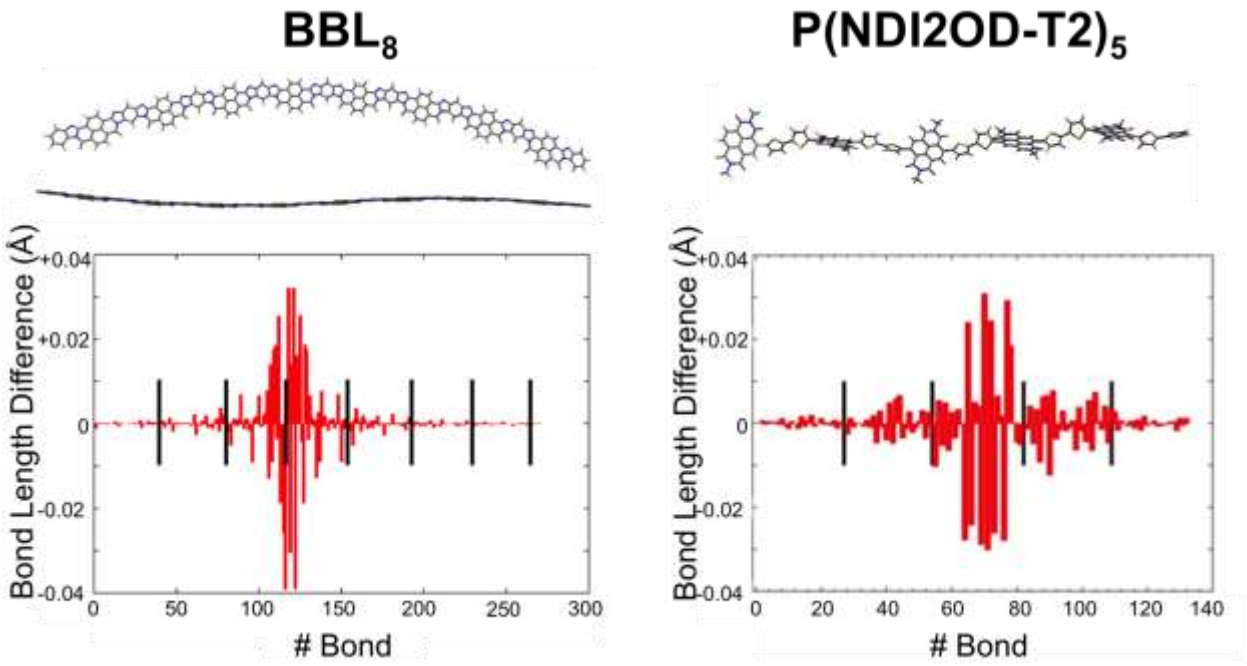
P(NDI2OD-T2), n = 5 ωB97X-D/6-31G* *Neutral state*	Energy eV	Oscillator Strength
S1	**2.8699**	**1.6842**
S2	2.9668	0.3425
S3	2.9881	0.0690
S4	3.0353	0.1274
S5	3.1241	0.0901
S6	3.1673	0.0058
S7	3.1865	0.0065
S8	3.2017	0.0106
S9	3.2411	0.0033
S10	3.7903	0.6863

P(NDI2OD-T2), n = 5 UωB97X-D/6-31G* *Charged (-1) state*	Energy eV	Oscillator Strength
D1	1.1769	0.0896
D2	1.2498	0.0007
D3	1.2745	0.0026
D4	1.3156	0.0396
D5	1.6840	0.0112
D6	1.8752	0.0010
D7	**1.9361**	**0.2908**
D8	2.0471	0.0000
D9	2.0691	0.0000
D10	2.2204	0.0005
D11	2.2803	0.0988
D12	2.3114	0.0498
D13	**2.3385**	**0.7057**
D14	2.4377	0.0169
D15	2.4778	0.0008
D16	2.4896	0.3026
D17	2.5431	0.0085
D18	2.5680	0.0000
D19	2.5806	0.0000

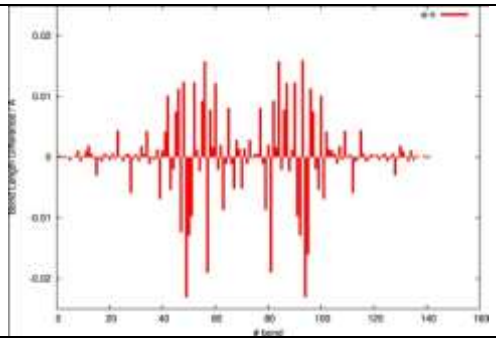
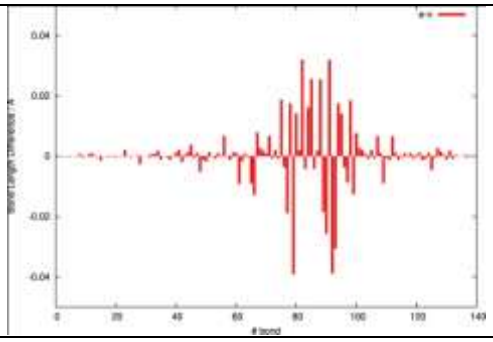
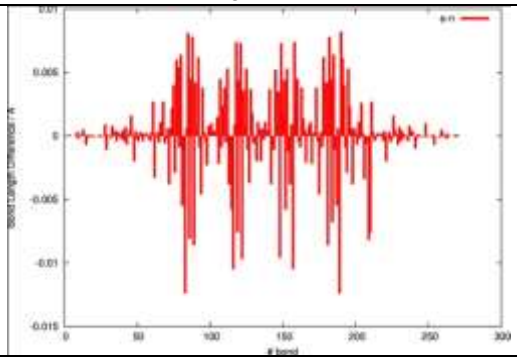
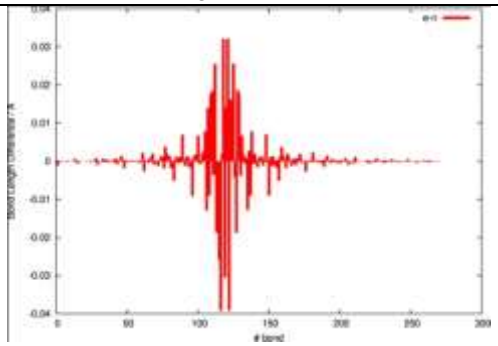
Computed DFT energy difference ΔE = E(UDFT-BS) – E(UDFT) between the unrestricted (UDFT) and the unrestricted – broken symmetry (UDFT-BS) solution for the BBL and P(NDI2OD-T2) oligomers investigated.

	BBL_n				$P(NDI2OD-T2)_n$
n	1	2	4	8	5
ΔE / eV	0.00	0.00	-0.27	-0.42	0.00

Comparison between the computed polaron structural relaxations (i.e. bond length difference) for BBL_8 (UDFT-BS) and $P(NDI2OD\text{-}T2)_5$ (UDFT). Bond length difference is computed as the difference between each bond in the charged and in the neutral state.



Comparison between the computed polaron structural relaxations at the UDFT and UDFT-BS levels, for BBL_4 and BBL_8. Structural relaxations are evaluated as bond length differences (Å) between the charged and the neutral optimized structures (C-H bonds are omitted from the analysis).

BBL_4 - *UDFT*	BBL_4 – *UDFT-BS*
	
BBL_8 - *UDFT*	BBL_8 – *UDFT-BS*
	

DFT optimized molecular structures: Cartesian coordinates (Å)

BBL, n = 1, ωB97X-D/6-31G*, neutral state

C	-2.555280	3.432870	0.189904
C	-3.178680	2.120154	0.142830
C	-2.332278	0.991721	-0.023268
C	-0.923379	1.129248	-0.140545
C	-0.276879	2.470689	-0.093445
N	-1.164064	3.533226	0.071632
C	-2.904131	-0.299942	-0.073322
C	-4.312601	-0.441057	0.043543
C	-5.112169	0.672077	0.204175
C	-4.544179	1.955020	0.253909
C	-2.054748	-1.426253	-0.239519
C	-2.613068	-2.806275	-0.297766
N	-4.000321	-2.872930	-0.177469
C	-4.865273	-1.784712	-0.012490
C	-0.122920	0.019991	-0.300953
C	-0.691536	-1.264354	-0.350709
O	-1.935230	-3.801833	-0.438661
C	-4.811241	-4.010340	-0.193870
O	0.919329	2.645736	-0.187775
C	-0.867993	4.896092	0.152481
H	-5.170728	2.831510	0.380103
H	-6.185320	0.539806	0.291258
H	0.949612	0.156591	-0.387733
H	-0.068591	-2.143321	-0.476742
N	-6.113638	-2.129924	0.073969
C	-6.117062	-3.516928	-0.035770
N	-3.142213	4.581709	0.333798
C	-2.115719	5.520762	0.314877
C	-2.194821	6.908072	0.431544
C	-1.009778	7.627788	0.380981
C	0.228462	6.985669	0.218119
C	0.327391	5.604626	0.100134
H	1.275959	5.099433	-0.025708
H	1.134147	7.583169	0.183229
H	-1.037632	8.709339	0.468866
H	-3.156425	7.393824	0.557009
C	-7.199423	-4.395807	-0.006828
C	-4.529587	-5.365629	-0.327159
C	-5.620663	-6.225549	-0.296006
C	-6.933029	-5.750921	-0.138761
H	-8.208938	-4.018487	0.115153
H	-7.753898	-6.460915	-0.120342
H	-5.452408	-7.293336	-0.396107
H	-3.514429	-5.720211	-0.447793

E = -1367.10698241 Hartree

BBL, n = 1, ωB97X-D/6-31G*, charged (-1) state

C	-2.571524	3.419096	0.190382
C	-3.180586	2.118018	0.142814
C	-2.329734	0.999484	-0.022974
C	-0.917873	1.140394	-0.140083
C	-0.285550	2.444686	-0.094307
N	-1.184946	3.518447	0.072305
C	-2.908170	-0.307009	-0.073793
C	-4.312311	-0.438176	0.043407
C	-5.128959	0.693220	0.207119
C	-4.571172	1.953078	0.256100
C	-2.059336	-1.437782	-0.240386
C	-2.599758	-2.782313	-0.297694
N	-4.003461	-2.847643	-0.175280
C	-4.866043	-1.763480	-0.011102
C	-0.108736	-0.002901	-0.304056
C	-0.664994	-1.259299	-0.352934
O	-1.948515	-3.814149	-0.438365
C	-4.806078	-3.983296	-0.192122
O	0.919478	2.663739	-0.186578
C	-0.884616	4.874031	0.152186
H	-5.187219	2.837356	0.382020
H	-6.200802	0.547998	0.293020
H	0.963098	0.141429	-0.390005
H	-0.048296	-2.142966	-0.478883
N	-6.130555	-2.118348	0.075806
C	-6.119329	-3.494102	-0.034037
N	-3.162191	4.586270	0.336306
C	-2.134226	5.507006	0.315729
C	-2.192470	6.899562	0.431113
C	-1.003352	7.612401	0.379462
C	0.231617	6.962434	0.215908
C	0.313981	5.579894	0.099128
H	1.253834	5.058951	-0.027419
H	1.143366	7.552528	0.179748
H	-1.025545	8.695634	0.467116
H	-3.150422	7.394517	0.557252
C	-7.191493	-4.391700	-0.007557
C	-4.520268	-5.339119	-0.325351
C	-5.601289	-6.212262	-0.296128
C	-6.917256	-5.745281	-0.139550
H	-8.205438	-4.023245	0.113772
H	-7.735657	-6.460453	-0.121709
H	-5.423305	-7.279504	-0.396724
H	-3.499271	-5.676751	-0.444884

E = -1367.18798960 Hartree

BBL, n = 2, ωB97X-D/6-31G*, neutral state

C	13.403365	-0.860643	-0.000263
C	12.316794	-1.723108	0.000685
C	11.041741	-1.158280	0.000232
C	10.887036	0.238031	-0.001122
C	11.967148	1.114083	-0.002109
C	13.229482	0.532833	-0.001656
N	9.805069	-1.795087	0.001014
C	8.929384	-0.837054	0.000190
N	9.504086	0.438979	-0.001138
C	7.481656	-0.964874	0.000490
C	6.712406	0.228911	-0.000225
C	7.326712	1.509831	-0.001345
C	8.810713	1.648918	-0.001902
C	6.858268	-2.195968	0.001465
C	5.457504	-2.283158	0.001698
C	4.686542	-1.138423	0.001047
C	5.302024	0.141169	0.000138
C	4.534216	1.336164	-0.000418
C	3.045173	1.291515	0.000066
N	2.505646	0.004635	0.000922
C	3.234111	-1.191397	0.001119
C	1.157178	-0.360094	0.000909
C	1.176472	-1.777657	0.001239
N	2.485008	-2.249758	0.001290
C	6.558111	2.652991	-0.001949
C	5.155021	2.565628	-0.001435
C	0.000035	-2.517219	0.001262
C	-1.176389	-1.777667	0.000958
C	-1.157178	-0.360088	0.000722
C	0.000015	0.407253	0.000702
O	2.341203	2.278238	-0.000190
O	9.387137	2.715652	-0.003009
N	-2.484970	-2.249794	0.000609
C	-3.234112	-1.191452	0.000622
C	-4.686552	-1.138486	0.000279

C	-5.302029	0.141109	0.000875
C	-4.534205	1.336095	0.001607
C	-3.045195	1.291453	0.001510
N	-2.505615	0.004544	0.000727
C	-5.457541	-2.283205	-0.000581
C	-6.858303	-2.195994	-0.000915
C	-7.481676	-0.964896	-0.000315
C	-6.712408	0.228877	0.000684
C	-7.326699	1.509810	0.001519
C	-8.810698	1.648923	0.001484
N	-9.504085	0.438984	0.000312
C	-8.929401	-0.837052	-0.000850
C	-10.887036	0.238057	-0.000696
C	-11.041759	-1.158252	-0.002368
N	-9.805097	-1.795075	-0.002376
C	-5.154998	2.565572	0.002347
C	-6.558088	2.652956	0.002363
C	-12.316819	-1.723069	-0.003896
C	-13.403378	-0.860596	-0.003641
C	-13.229479	0.532880	-0.001867
C	-11.967142	1.114117	-0.000357
O	-9.387114	2.715657	0.002324
O	-2.341278	2.278218	0.002157
H	-7.468234	-3.093094	-0.001669
H	-4.963432	-3.248852	-0.001004
H	-7.054183	3.617435	0.003005
H	-4.542376	3.460772	0.002901
H	-11.823259	2.186437	0.001043
H	-14.104055	1.176031	-0.001680
H	-14.409253	-1.268793	-0.004868
H	-12.438894	-2.800757	-0.005306
H	4.963390	-3.248803	0.002392
H	7.468184	-3.093078	0.002011
H	4.542400	3.460828	-0.001838
H	7.054214	3.617465	-0.002832
H	-0.000003	1.486774	0.000606
H	0.000062	-3.600490	0.001341
H	12.438864	-2.800797	0.001806
H	14.409236	-1.268850	0.000076
H	14.104066	1.175974	-0.002368
H	11.823266	2.186403	-0.003194

E = -2502.04817843 Hartree

BBL, n = 2, ωB97X-D/6-31G*, charged (-1) state

C	13.390000	-0.837450	0.000203
C	12.308804	-1.706844	0.000326
C	11.025454	-1.156143	0.000068
C	10.862514	0.241919	-0.000298
C	11.938956	1.123770	-0.000442
C	13.207212	0.555138	-0.000181
N	9.799614	-1.801266	0.000140
C	8.912367	-0.840924	-0.000136
N	9.482297	0.434714	-0.000482
C	7.473007	-0.965492	-0.000114
C	6.708227	0.228092	-0.000222
C	7.321769	1.510995	-0.000491
C	8.782898	1.652422	-0.000801
C	6.845334	-2.207823	0.000100
C	5.457400	-2.296755	0.000188
C	4.679806	-1.141817	0.000128
C	5.290149	0.137946	-0.000054
C	4.516154	1.331020	-0.000068
C	3.046576	1.288334	0.000185
N	2.507418	-0.001197	0.000290
C	3.236045	-1.195820	0.000201
C	1.160093	-0.365575	0.000281
C	1.179719	-1.786036	0.000261
N	2.481783	-2.260690	0.000192
C	6.534915	2.660961	-0.000513
C	5.147837	2.572986	-0.000300
C	0.000001	-2.523111	0.000265
C	-1.179717	-1.786035	0.000303
C	-1.160091	-0.365574	0.000367
C	0.000001	0.398280	0.000351
O	2.326091	2.275059	0.000019
O	9.384030	2.714576	-0.000646
N	-2.481782	-2.260688	0.000243
C	-3.236044	-1.195819	0.000326
C	-4.679805	-1.141817	0.000239
C	-5.290149	0.137946	0.000338
C	-4.516154	1.331020	0.000588
C	-3.046575	1.288334	0.000852
N	-2.507417	-0.001196	0.000481
C	-5.457400	-2.296753	-0.000020
C	-6.845334	-2.207822	-0.000177
C	-7.473007	-0.965492	-0.000096
C	-6.708227	0.228092	0.000163
C	-7.321770	1.510995	0.000255
C	-8.782899	1.652421	0.000044
N	-9.482298	0.434714	-0.000096
C	-8.912368	-0.840924	-0.000266
C	-10.862515	0.241919	-0.000276
C	-11.025455	-1.156143	-0.000594
N	-9.799614	-1.801265	-0.000585
C	-5.147837	2.572985	0.000654
C	-6.534916	2.660960	0.000505
C	-12.308804	-1.706845	-0.000887
C	-13.390001	-0.837451	-0.000841
C	-13.207213	0.555137	-0.000503
C	-11.938957	1.123769	-0.000217
O	-9.384030	2.714575	0.000401
O	-2.326092	2.275060	0.000497
H	-7.461403	-3.100973	-0.000382
H	-4.958186	-3.259728	-0.000102
H	-7.032581	3.624885	0.000576
H	-4.528689	3.463497	0.000858
H	-11.781142	2.194200	0.000040
H	-14.076918	1.205832	-0.000476
H	-14.399069	-1.240019	-0.001078
H	-12.439593	-2.784045	-0.001160
H	4.958186	-3.259730	0.000330
H	7.461403	-3.100974	0.000191
H	4.528689	3.463498	-0.000307
H	7.032580	3.624886	-0.000730
H	0.000001	1.477628	0.000420
H	0.000001	-3.606822	0.000214
H	12.439594	-2.784045	0.000631
H	14.399069	-1.240017	0.000405
H	14.076917	1.205833	-0.000278
H	11.781140	2.194201	-0.000755

E = -2502.12481349 Hartree

BBL, n = 4, ωB97X-D/6-31G*, neutral state

C	-0.000007	-0.556437	0.691381
C	1.157124	-1.313114	0.564324
C	1.176518	-2.712009	0.335018
C	-0.000009	-3.442367	0.219253
C	-1.176525	-2.712008	0.335049
C	-1.157141	-1.313110	0.564336
N	2.484981	-3.173907	0.236178
C	3.233497	-2.126356	0.389912

N	2.505106	-0.949065	0.600191
C	4.685040	-2.064996	0.345675
C	5.298763	-0.795283	0.511434
C	4.531340	0.379690	0.730976
C	3.043723	0.324811	0.786509
C	6.707107	-0.695948	0.450520
C	7.475493	-1.868896	0.226210
C	6.854383	-3.091866	0.074638
C	5.455663	-3.190295	0.134197
C	7.319262	0.575978	0.609170
C	8.799508	0.729475	0.536805
N	9.492622	-0.459202	0.304686
C	8.920001	-1.727822	0.152683
C	10.871796	-0.635674	0.170546
C	11.028265	-2.026534	-0.053488
N	9.792174	-2.664496	-0.055289
C	11.920728	0.272803	0.218802
C	13.159794	-0.321574	0.020495
C	13.354019	-1.707520	-0.206328
C	12.282996	-2.591926	-0.245584
N	14.704881	-1.991400	-0.377408
C	15.313696	-0.852113	-0.265245
N	14.447019	0.219756	-0.019454
C	16.740866	-0.601787	-0.373418
C	17.191758	0.735608	-0.218202
C	16.287249	1.800871	0.036445
C	14.822047	1.553875	0.147221
C	18.573389	1.014051	-0.321466
C	19.478094	-0.049271	-0.580349
C	19.013196	-1.340346	-0.726841
C	17.641623	-1.617182	-0.622381
C	19.024159	2.352081	-0.164723
C	20.472480	2.690857	-0.265399
N	21.303902	1.601374	-0.524501
C	20.890857	0.273986	-0.685879
C	22.692924	1.593057	-0.680809
C	23.013079	0.247407	-0.927549
N	21.869714	-0.544454	-0.923221
C	23.653831	2.597043	-0.631488
C	24.969011	2.200418	-0.842727
C	25.307411	0.860280	-1.091493
C	24.338820	-0.131454	-1.137224
C	16.750911	3.089568	0.184292
C	18.125671	3.366050	0.083862
C	5.150486	1.599876	0.888180
C	6.551512	1.698797	0.826473
O	20.911916	3.813610	-0.137645
O	14.005566	2.423602	0.361638
O	9.374173	1.789229	0.662248
O	2.339747	1.294112	0.970681
N	-2.484994	-3.173915	0.236274
C	-3.233503	-2.126370	0.390019
N	-2.505112	-0.949069	0.600246
C	-3.043724	0.324804	0.786598
C	-4.531341	0.379685	0.731079
C	-5.298769	-0.795292	0.511568
C	-4.685049	-2.065007	0.345812
C	-6.707113	-0.695957	0.450675
C	-7.475503	-1.868909	0.226390
C	-6.854397	-3.091880	0.074819
C	-5.455675	-3.190307	0.134357
C	-7.319268	0.575971	0.609316
C	-6.551515	1.698794	0.826579
C	-5.150487	1.599874	0.888267
C	-8.799517	0.729460	0.537011
N	-9.492631	-0.459214	0.304865
C	-8.920011	-1.727834	0.152866
N	-9.792187	-2.664511	-0.055086
C	-11.028274	-2.026544	-0.053305
C	-10.871801	-0.635678	0.170684
C	-12.283007	-2.591938	-0.245392
C	-13.354025	-1.707527	-0.206175
C	-13.159797	-0.321573	0.020598
C	-11.920731	0.272805	0.218900
N	-14.447020	0.219759	-0.019380
C	-15.313699	-0.852115	-0.265140
N	-14.704887	-1.991411	-0.377248
C	-14.822047	1.553886	0.147241
C	-16.287244	1.800886	0.036412
C	-17.191754	0.735616	-0.218202
C	-16.740865	-0.601789	-0.373345
C	-18.573380	1.014060	-0.321513
C	-19.478085	-0.049270	-0.580359
C	-19.013191	-1.340356	-0.726773
C	-17.641621	-1.617192	-0.622276
C	-19.024148	2.352101	-0.164845
C	-18.125661	3.366076	0.083714
C	-16.750903	3.089593	0.184183
C	-20.472464	2.690881	-0.265588
N	-21.303888	1.601385	-0.524628
C	-20.890846	0.273986	-0.685924
N	-21.869702	-0.544464	-0.923232
C	-23.013066	0.247399	-0.927602
C	-22.692909	1.593062	-0.680935
C	-24.338807	-0.131472	-1.137259
C	-25.307397	0.860266	-1.091585
C	-24.968995	2.200417	-0.842895
C	-23.653814	2.597052	-0.631675
O	-2.339750	1.294111	0.970741
O	-9.374173	1.789233	0.662328
O	-14.005557	2.423634	0.361541
O	-20.911909	3.813625	-0.137786
H	-19.724862	-2.134721	-0.924477
H	-17.271077	-2.630128	-0.738123
H	-18.498811	4.377936	0.199933
H	-16.037237	3.883136	0.377977
H	-23.385150	3.627335	-0.439915
H	-25.754356	2.949096	-0.814920
H	-26.348935	0.599554	-1.251461
H	-24.586696	-1.169942	-1.327985
H	-7.463565	-3.972930	-0.096293
H	-4.963110	-4.148595	0.009210
H	-7.046365	2.656652	0.945125
H	-4.538525	2.479619	1.055637
H	-11.785026	1.330217	0.388388
H	-12.417724	-3.652432	-0.419733
H	4.963098	-4.148583	0.009053
H	7.463548	-3.972917	-0.096485
H	4.538524	2.479617	1.055573
H	7.046366	2.656653	0.945021
H	0.000004	0.509386	0.862621
H	-0.000002	-4.510566	0.039291
H	17.271077	-2.630110	-0.738287
H	19.724866	-2.134705	-0.924571
H	16.037244	3.883103	0.378114
H	18.498824	4.377902	0.200136
H	11.785025	1.330211	0.388319
H	12.417710	-3.652413	-0.419964
H	24.586709	-1.169913	-1.328011
H	26.348948	0.599574	-1.251383
H	25.754374	2.949093	-0.814707
H	23.385166	3.627314	-0.439668

E = -4771.93058488 Hartree

BBL, n = 4, UωB97X-D/6-31G*, charged (-1) state

C	0.000001	-0.580836	0.678295

C	1.159940	-1.334317	0.552541
C	1.179567	-2.736127	0.323679
C	0.000000	-3.464328	0.208890
C	-1.179566	-2.736126	0.323679
C	-1.159939	-1.334317	0.552541
N	2.481484	-3.200910	0.224718
C	3.235093	-2.147012	0.378101
N	2.506878	-0.970737	0.587624
C	4.677869	-2.085341	0.334168
C	5.287143	-0.815862	0.500673
C	4.514214	0.357503	0.719837
C	3.045393	0.305428	0.774028
C	6.703241	-0.714824	0.440203
C	7.466159	-1.888618	0.216241
C	6.839810	-3.122500	0.062286
C	5.454103	-3.221360	0.120574
C	7.314739	0.558714	0.599504
C	8.771699	0.713720	0.529600
N	9.470458	-0.484688	0.296188
C	8.901349	-1.752580	0.143342
C	10.845444	-0.653394	0.164807
C	11.009660	-2.047495	-0.060063
N	9.784992	-2.692376	-0.064735
C	11.890815	0.260790	0.215522
C	13.134612	-0.323525	0.019962
C	13.337211	-1.707228	-0.206658
C	12.272253	-2.599499	-0.248918
N	14.692094	-1.982309	-0.374758
C	15.294976	-0.840764	-0.261208
N	14.422515	0.227510	-0.017199
C	16.721827	-0.589355	-0.367209
C	17.171964	0.748924	-0.212362
C	16.261929	1.809182	0.039638
C	14.793055	1.556848	0.148647
C	18.553094	1.031492	-0.313226
C	19.460408	-0.029514	-0.569384
C	18.996799	-1.321659	-0.715535
C	17.626231	-1.602612	-0.613747
C	18.998072	2.371781	-0.156522
C	20.442474	2.714622	-0.254434
N	21.279116	1.626137	-0.511296
C	20.871972	0.296689	-0.672499
C	22.667842	1.624690	-0.664391
C	22.995052	0.280201	-0.909479
N	21.856395	-0.517610	-0.907192
C	23.624090	2.633120	-0.613811
C	24.942212	2.244012	-0.821945
C	25.287550	0.905604	-1.069047
C	24.323437	-0.090883	-1.116007
C	16.719476	3.099708	0.187403
C	18.093133	3.381498	0.089441
C	5.144265	1.589740	0.879162
C	6.529352	1.688637	0.818938
O	20.884044	3.837633	-0.127453
O	13.983282	2.433797	0.362209
O	9.373400	1.767286	0.652836
O	2.325901	1.274972	0.958078
N	-2.481483	-3.200909	0.224720
C	-3.235092	-2.147011	0.378103
N	-2.506877	-0.970736	0.587623
C	-3.045392	0.305429	0.774027
C	-4.514214	0.357503	0.719840
C	-5.287143	-0.815862	0.500678
C	-4.677869	-2.085340	0.334172
C	-6.703241	-0.714824	0.440211
C	-7.466160	-1.888619	0.216249
C	-6.839810	-3.122500	0.062292
C	-5.454103	-3.221360	0.120579
C	-7.314740	0.558713	0.599515
C	-6.529352	1.688636	0.818947
C	-5.144265	1.589739	0.879167
C	-8.771700	0.713718	0.529617
N	-9.470459	-0.484689	0.296199
C	-8.901350	-1.752580	0.143350
N	-9.784992	-2.692376	-0.064729
C	-11.009660	-2.047495	-0.060058
C	-10.845445	-0.653394	0.164813
C	-12.272253	-2.599498	-0.248915
C	-13.337211	-1.707228	-0.206656
C	-13.134613	-0.323524	0.019965
C	-11.890816	0.260790	0.215527
N	-14.422516	0.227510	-0.017197
C	-15.294976	-0.840763	-0.261208
N	-14.692094	-1.982308	-0.374757
C	-14.793056	1.556848	0.148648
C	-16.261929	1.809183	0.039635
C	-17.171964	0.748925	-0.212366
C	-16.721827	-0.589354	-0.367211
C	-18.553094	1.031493	-0.313233
C	-19.460407	-0.029513	-0.569389
C	-18.996798	-1.321659	-0.715538
C	-17.626231	-1.602612	-0.613748
C	-18.998071	2.371783	-0.156531
C	-18.093133	3.381499	0.089433
C	-16.719476	3.099709	0.187398
C	-20.442473	2.714624	-0.254451
N	-21.279115	1.626138	-0.511305
C	-20.871972	0.296689	-0.672503
N	-21.856395	-0.517611	-0.907192
C	-22.995052	0.280200	-0.909477
C	-22.667842	1.624690	-0.664394
C	-24.323438	-0.090886	-1.115999
C	-25.287551	0.905601	-1.069039
C	-24.942213	2.244010	-0.821942
C	-23.624090	2.633120	-0.613814
O	-2.325902	1.274973	0.958080
O	-9.373400	1.767286	0.652842
O	-13.983282	2.433798	0.362208
O	-20.884044	3.837634	-0.127458
H	-19.710524	-2.114868	-0.911336
H	-17.257185	-2.616017	-0.729550
H	-18.461241	4.395298	0.205703
H	-16.000322	3.888777	0.379028
H	-23.348132	3.661709	-0.423142
H	-25.723563	2.997041	-0.792709
H	-26.330766	0.649457	-1.226828
H	-24.576863	-1.128338	-1.305679
H	-7.454163	-4.000202	-0.108550
H	-4.955829	-4.176642	-0.004118
H	-7.025736	2.645800	0.938136
H	-4.526270	2.465063	1.046346
H	-11.741696	1.316069	0.385891
H	-12.416007	-3.658911	-0.423626
H	4.955829	-4.176643	-0.004121
H	7.454162	-4.000202	-0.108556
H	4.526271	2.465064	1.046342
H	7.025736	2.645801	0.938125
H	0.000001	0.484998	0.848350
H	0.000000	-4.532985	0.029165
H	17.257185	-2.616017	-0.729550
H	19.710525	-2.114868	-0.911335
H	16.000322	3.888776	0.379033
H	18.461242	4.395297	0.205714
H	11.741695	1.316070	0.385884
H	12.416007	-3.658912	-0.423629
H	24.576862	-1.128336	-1.305691
H	26.330764	0.649460	-1.226841
H	25.723562	2.997042	-0.792713
H	23.348132	3.661709	-0.423135

E = -4772.01136729 Hartree

BBL, n = 4, UωB97X-D/6-31G* broken symmetry (BS), charged (-1) state

C	-0.030736	-0.593289	0.673982
C	1.133815	-1.337918	0.552536
C	1.162160	-2.736389	0.325699
C	-0.008161	-3.478008	0.208115
C	-1.198730	-2.764535	0.317658
C	-1.185199	-1.357264	0.545233
N	2.475977	-3.188864	0.230346
C	3.219877	-2.138429	0.383662
N	2.485665	-0.963038	0.590518
C	4.669922	-2.080603	0.339663
C	5.287849	-0.811550	0.504307
C	4.515664	0.359399	0.721207
C	3.021239	0.302313	0.776401
C	6.696414	-0.711038	0.444727
C	7.464488	-1.883714	0.222934
C	6.840009	-3.106532	0.072277
C	5.442467	-3.206475	0.130408
C	7.304912	0.563121	0.602740
C	8.779818	0.718503	0.532473
N	9.476592	-0.472687	0.301791
C	8.907419	-1.743500	0.150532
C	10.854919	-0.643065	0.170290
C	11.017385	-2.034585	-0.051763
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H	38.237871	7.509409	-0.240250
H	40.506137	8.579598	-0.022951
H	34.713769	4.019021	-0.260417
H	36.499908	-0.659642	0.633683
H	47.720982	4.649440	1.618512
H	49.009543	6.787162	1.548876
H	47.874448	8.927897	1.106194
H	45.412545	9.020701	0.714397

E = -9311.69545819 Hartree

BBL, n = 8, (U)ωB97X-D/6-31G*, charged (-1) state

C	0.006309	-3.539721	-0.369450
C	1.164534	-4.303295	-0.304178
C	1.184958	-5.704421	-0.081142
C	0.009207	-6.424838	0.094602
C	-1.167858	-5.687506	0.038987
C	-1.150122	-4.287220	-0.188954
N	2.511138	-3.951172	-0.417626
C	3.239671	-5.135732	-0.258728
N	2.489989	-6.179816	-0.062438
C	4.687528	-5.089119	-0.313987
C	5.299643	-3.825469	-0.517795
C	4.529230	-2.641642	-0.675241
C	3.050263	-2.679468	-0.629233
C	5.156128	-1.422624	-0.870255
C	6.551478	-1.339579	-0.911481
C	7.328607	-2.475676	-0.758545
C	6.713169	-3.741552	-0.560644
C	7.479829	-4.924249	-0.399437
C	8.923442	-4.800861	-0.432896
N	9.497606	-3.539041	-0.625499
C	8.801423	-2.339192	-0.799728
N	9.800376	-5.750499	-0.290829
C	11.036836	-5.125289	-0.383488
C	10.880227	-3.730808	-0.594791
C	11.935583	-2.836128	-0.719082
C	13.180076	-3.443160	-0.610950
C	13.373661	-4.832583	-0.398455
C	12.296336	-5.703611	-0.282649
N	14.473882	-2.917569	-0.663591
C	15.341915	-4.000002	-0.479960
N	14.726746	-5.134987	-0.324364
C	16.771645	-3.769580	-0.470872
C	17.226998	-2.438315	-0.654591
C	16.318818	-1.362385	-0.846209
C	14.854268	-1.587759	-0.855006
C	16.793511	-0.073227	-1.024138
C	18.167456	0.184600	-1.014387
C	19.076702	-0.843722	-0.825203
C	18.619795	-2.176936	-0.642298
C	19.521435	-3.253831	-0.443648
C	20.936866	-2.952869	-0.421725
N	21.355855	-1.630296	-0.603468
C	20.520072	-0.524273	-0.812843
C	22.747952	-1.647154	-0.521152
C	23.069711	-3.011149	-0.291400
N	21.920583	-3.785510	-0.238906
C	23.687144	-0.628008	-0.618766
C	24.992750	-1.075109	-0.463753
C	25.349482	-2.426796	-0.231930
C	24.387914	-3.425686	-0.142977
N	26.729968	-2.555424	-0.110534
C	27.203333	-1.357820	-0.255997
N	26.214091	-0.391551	-0.478098
C	26.433995	0.970353	-0.666150
C	27.868388	1.379858	-0.605685
C	28.893961	0.424950	-0.375367
C	28.597790	-0.952836	-0.200330
C	30.238236	0.856491	-0.312694
C	31.261832	-0.098295	-0.076054
C	30.947261	-1.432545	0.086004
C	29.612532	-1.861195	0.023507
C	30.529798	2.236255	-0.483711
C	29.516200	3.141183	-0.711265
C	28.179055	2.711189	-0.772233
C	31.928818	2.737672	-0.412788
N	32.885284	1.749480	-0.167058
C	32.630754	0.382759	0.001571
N	33.700456	-0.315049	0.229137
C	34.747216	0.600379	0.225771
C	34.264515	1.910486	-0.021674
C	36.098247	0.356041	0.438476
C	36.926553	1.471069	0.395473
C	36.409202	2.766391	0.143623
C	35.066408	3.043055	-0.076053
N	38.303702	1.521750	0.586322
C	38.623439	2.771815	0.462289
N	37.529418	3.601579	0.188039
C	37.578323	4.983159	0.003209
C	38.940181	5.576140	0.133334
C	40.068611	4.762029	0.418473
C	39.947426	3.357419	0.586205
C	41.341173	5.364484	0.539377
C	42.469130	4.550651	0.824931
C	42.323548	3.187399	0.982820
C	41.059948	2.589199	0.863441
C	41.460551	6.770327	0.373317
C	40.349989	7.536439	0.094622
C	39.084096	6.936638	-0.026469
C	42.782151	7.447028	0.497970
N	43.846209	6.589870	0.779598
C	43.762207	5.202578	0.943115
N	44.907236	4.643853	1.191966
C	45.826631	5.687370	1.201946
C	45.194461	6.916167	0.948390
C	47.203158	5.638820	1.420507
C	47.904783	6.834731	1.377742
C	47.255649	8.053819	1.124007
C	45.885169	8.122218	0.903198
C	17.676213	-4.803004	-0.282909
C	19.048189	-4.545218	-0.268571
C	5.461258	-6.228594	-0.164282
C	6.855731	-6.145963	-0.207239
O	25.525139	1.749098	-0.858756
O	32.239297	3.901771	-0.549054
O	36.583349	5.631371	-0.239582
O	42.943150	8.642051	0.369238
O	20.981797	0.590361	-0.964095
O	14.030612	-0.706385	-1.011068
O	9.387463	-1.286063	-0.965418
O	2.337569	-1.702210	-0.757940
N	-2.470917	-6.144135	0.190409
C	-3.221768	-5.090007	0.065153
C	-4.667310	-5.023518	0.150694
C	-5.280262	-3.754480	-0.013228
C	-4.513471	-2.583204	-0.258006
C	-3.037074	-2.640038	-0.347122
N	-2.496361	-3.916432	-0.170793
C	-5.437443	-6.150269	0.388904
C	-6.829035	-6.050181	0.470957
C	-7.453783	-4.823628	0.315187
C	-6.690807	-3.653004	0.070012
C	-7.306806	-2.382453	-0.093089
C	-8.776120	-2.228657	-0.011450
N	-9.468670	-3.418539	0.231651
C	-8.894202	-4.684528	0.394113
C	-10.847750	-3.597180	0.355722
C	-11.002289	-4.988521	0.587921
N	-9.767878	-5.624370	0.604731
C	-12.258428	-5.556421	0.762651
C	-13.334520	-4.678842	0.694560
C	-13.142957	-3.292405	0.461515
C	-11.901737	-2.695272	0.283575
N	-14.684824	-4.973039	0.828471
C	-15.300353	-3.836504	0.686146
N	-14.435024	-2.759990	0.459847
C	-16.728556	-3.601183	0.733602
C	-17.185252	-2.271463	0.542161
C	-16.279420	-1.200143	0.316569
C	-14.816434	-1.430385	0.268918
C	-17.631009	-4.630405	0.952309
C	-19.002409	-4.370911	0.983969
C	-19.477193	-3.081692	0.797393
C	-18.577339	-2.007958	0.574637
C	-19.035557	-0.676817	0.380486
C	-20.478651	-0.357032	0.400506
N	-21.313190	-1.461847	0.620621
C	-20.893068	-2.782216	0.815288
C	-22.706291	-1.482807	0.679984
C	-23.027680	-2.846462	0.912325
N	-21.876926	-3.616340	0.990730
C	-24.347663	-3.266952	1.024367
C	-25.311446	-2.274761	0.893374

C	-24.954561	-0.922642	0.664469
C	-23.647181	-0.469103	0.548744
N	-26.178810	-0.248685	0.588287
C	-27.170319	-1.221202	0.769004
N	-26.695244	-2.413141	0.951175
C	-16.755246	0.087768	0.132689
C	-18.128349	0.348015	0.164610
C	-5.141128	-1.359147	-0.415201
C	-6.533538	-1.258842	-0.332830
C	-26.399330	1.109936	0.379016
C	-27.838422	1.505191	0.344553
C	-28.867374	0.541149	0.513526
C	-28.569523	-0.830484	0.729437
C	-30.217441	0.955967	0.462967
C	-30.510534	2.329205	0.248171
C	-29.493026	3.244688	0.091510
C	-28.150353	2.830700	0.138746
C	-31.245432	-0.009913	0.624041
C	-30.928657	-1.337065	0.833366
C	-29.588015	-1.748404	0.887527
C	-31.916681	2.810720	0.184231
N	-32.878258	1.810085	0.344038
C	-32.622379	0.449131	0.552629
N	-33.699799	-0.266436	0.654642
C	-34.754045	0.628808	0.508551
C	-34.267236	1.946105	0.313108
C	-35.075117	3.061215	0.133278
C	-36.429618	2.757400	0.157913
C	-36.952064	1.453213	0.345493
C	-36.116621	0.357777	0.528512
N	-37.560391	3.565518	0.008949
C	-38.665741	2.711761	0.108984
N	-38.342728	1.472185	0.307888
C	-40.003916	3.262875	-0.021305
C	-40.126444	4.660526	-0.239533
C	-38.985319	5.501930	-0.325744
C	-37.608670	4.944008	-0.197265
C	-41.413402	5.227923	-0.376045
C	-41.534499	6.626588	-0.593525
C	-40.411143	7.420528	-0.669023
C	-39.130683	6.855516	-0.534999
C	-42.554104	4.386292	-0.294706
C	-42.406962	3.030824	-0.081398
C	-41.129217	2.467605	0.056370
C	-42.871714	7.265564	-0.747691
N	-43.947826	6.381829	-0.661387
C	-43.861553	5.001635	-0.446813
N	-45.018200	4.413582	-0.410998
C	-45.948611	5.428046	-0.609949
C	-45.311100	6.669906	-0.769652
C	-46.011098	7.852059	-0.985294
C	-47.395897	7.745438	-1.037335
C	-48.050006	6.512869	-0.880127
C	-47.339376	5.341112	-0.664785
O	-20.941367	0.756151	0.241718
O	-13.994968	-0.553530	0.079471
O	-9.362333	-1.170542	-0.140730
O	-2.327463	-1.673917	-0.553513
O	-25.487713	1.896127	0.236047
O	-32.229059	3.968688	0.006346
O	-36.602027	5.615656	-0.265825
O	-43.034670	8.452593	-0.934583
H	-43.294519	2.409740	-0.024005
H	-41.007986	1.402658	0.222904
H	-40.533943	8.485326	-0.835080
H	-38.241187	7.473414	-0.595499
H	-45.498633	8.797255	-1.105898
H	-47.985439	8.641442	-1.204681
H	-49.133976	6.479008	-0.929901
H	-47.833036	4.383304	-0.541836
H	-31.731809	-2.056558	0.952335
H	-29.335183	-2.790419	1.050949
H	-29.746441	4.286714	-0.071226
H	-27.343648	3.544783	0.013240
H	-34.688893	4.058473	-0.013654
H	-36.503787	-0.643581	0.672722
H	-19.715894	-5.170588	1.151965
H	-17.250576	-5.636034	1.095378
H	-18.507540	1.353945	0.019692
H	-16.039654	0.884944	-0.037055
H	-23.385320	0.562956	0.371679
H	-24.607021	-4.304190	1.198418
H	-7.438881	-6.927539	0.658093
H	-4.940810	-7.106784	0.511398
H	-7.031150	-0.302799	-0.454302
H	-4.529437	-0.483186	-0.602187
H	-11.767143	-1.638972	0.106567
H	-12.391665	-6.616906	0.939262
H	4.965344	-7.180883	-0.010013
H	7.468491	-7.032949	-0.087085
H	4.541802	-0.536398	-0.987050
H	7.048241	-0.387041	-1.060768
H	0.004842	-2.473793	-0.539250
H	0.010456	-7.494133	0.269084
H	17.296715	-5.809611	-0.144287
H	19.763107	-5.347128	-0.118220
H	16.076072	0.727405	-1.167934
H	18.545448	1.192026	-1.151912
H	11.800252	-1.777171	-0.878792
H	12.430901	-6.765836	-0.117929
H	29.360739	-2.907907	0.155463
H	31.747166	-2.142718	0.266705
H	27.375377	3.418286	-0.946869
H	29.767918	4.188443	-0.839390
H	23.424917	0.404391	-0.793525
H	24.647210	-4.462174	0.035562
H	40.939560	1.518633	0.989539
H	43.201245	2.588633	1.201742
H	38.204534	7.532656	-0.245151
H	40.471188	8.607158	-0.028889
H	34.683667	4.034780	-0.263723
H	36.481212	-0.638689	0.631279
H	47.693327	4.691089	1.614799
H	48.977637	6.831429	1.543762
H	47.838065	8.969629	1.099254
H	45.375662	9.056408	0.707149

E = -9311.77140629 Hartree

BBL, n = 8, (U)ωB97X-D/6-31G* broken symmetry (BS), charged (-1) state

C	0.027004	-3.591898	0.356401
C	1.178675	-4.348841	0.172353
C	1.189965	-5.755870	-0.056589
C	0.000301	-6.477187	-0.107012
C	-1.167177	-5.743749	0.072546
C	-1.137228	-4.344534	0.295224
N	2.518079	-3.985961	0.151881
C	3.242272	-5.156405	-0.084600
N	2.478629	-6.219945	-0.209664
C	4.672431	-5.080869	-0.168634
C	5.275289	-3.810588	-0.003445
C	4.507363	-2.638625	0.242122
C	3.060248	-2.693198	0.329503
C	5.150864	-1.395023	0.402580
C	6.520332	-1.295076	0.321825
C	7.313301	-2.434463	0.076797
C	6.698368	-3.706606	-0.087487
C	7.454305	-4.878027	-0.333362
C	8.880427	-4.746577	-0.412733
N	9.452434	-3.483196	-0.248887
C	8.753878	-2.279624	-0.002412
N	9.768918	-5.692302	-0.626692
C	10.987730	-5.049784	-0.606758
C	10.824641	-3.653364	-0.371209
C	11.872534	-2.742337	-0.295580
C	13.118834	-3.326814	-0.472468
C	13.320742	-4.709586	-0.707482
C	12.254977	-5.599227	-0.779762
N	14.412549	-2.781576	-0.467549
C	15.285152	-3.853836	-0.694804
N	14.678240	-4.989888	-0.839337

C	16.716416	-3.618943	-0.741496
C	17.176538	-2.288554	-0.548694
C	16.267030	-1.222610	-0.322836
C	14.789541	-1.460689	-0.276353
C	16.731702	0.060575	-0.137656
C	18.111350	0.327464	-0.168512
C	19.016783	-0.689607	-0.384083
C	18.564134	-2.022211	-0.579997
C	19.468367	-3.092417	-0.803293
C	20.886853	-2.787853	-0.820011
N	21.303270	-1.464986	-0.623949
C	20.466280	-0.364850	-0.403508
C	22.697650	-1.481954	-0.682628
C	23.022298	-2.843522	-0.915570
N	21.870786	-3.616656	-0.995010
C	23.635899	-0.466401	-0.550338
C	24.944335	-0.917764	-0.665932
C	25.304082	-2.268733	-0.895523
C	24.341653	-3.262652	-1.027496
N	26.687752	-2.404550	-0.952977
C	27.160288	-1.211624	-0.769869
N	26.166632	-0.241581	-0.588922
C	26.383713	1.118255	-0.378610
C	27.821510	1.516818	-0.343433
C	28.852570	0.555011	-0.512682
C	28.558445	-0.817245	-0.729520
C	30.201597	0.973039	-0.461410
C	31.232006	0.009704	-0.622687
C	30.918783	-1.318067	-0.832889
C	29.579113	-1.732618	-0.887769
C	30.491491	2.346787	-0.245718
C	29.472073	3.259964	-0.088796
C	28.130298	2.842902	-0.136707
C	31.896859	2.831635	-0.181047
N	32.860678	1.833486	-0.341272
C	32.607868	0.472080	-0.550548
N	33.686717	-0.241101	-0.652608
C	34.739072	0.656299	-0.505837
C	34.249453	1.972447	-0.309932
C	36.102166	0.387956	-0.525606
C	36.935252	1.485010	-0.341919
C	36.410101	2.788100	-0.153934
C	35.054966	3.089173	-0.129468
N	38.325811	1.506721	-0.304016
C	38.646246	2.746873	-0.104561
N	37.539186	3.598375	-0.004431
C	37.584733	4.977020	0.202181
C	38.960253	5.537581	0.331022
C	40.103018	4.698372	0.244770
C	39.983274	3.300558	0.026177
C	41.388885	5.268152	0.381585
C	42.531181	4.428674	0.300232
C	42.386706	3.072972	0.086607
C	41.110058	2.507403	-0.051508
C	41.507334	6.666999	0.599366
C	40.382467	7.458788	0.674894
C	39.103066	6.891405	0.540595
C	42.843385	7.308425	0.753810
N	43.921147	6.426702	0.667544
C	43.837445	5.046410	0.452676
N	44.995159	4.460478	0.416919
C	45.923678	5.476598	0.616225
C	45.283878	6.717257	0.776078
C	47.314591	5.392168	0.671263
C	48.023037	6.565176	0.886932
C	47.366655	7.796527	1.044267
C	45.981667	7.900650	0.992043
C	17.619190	-4.641233	-0.959938
C	18.995380	-4.376730	-0.990391
C	5.452825	-6.224593	-0.411650
C	6.824343	-6.124310	-0.492853
O	25.469286	1.900859	-0.235714
O	32.205923	3.990255	-0.002320
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C	-24.410923	-0.496178	0.309597
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O	-33.016758	4.517126	2.055244
C	-29.804284	-1.846561	-3.102809
C	-31.226976	5.048899	3.960145
H	-33.666270	3.189469	0.027929
H	-33.287626	1.475695	-1.774841
H	-29.814435	-2.823594	-2.618965
H	-30.610012	-1.779205	-3.826614
H	-28.840230	-1.713217	-3.591866
H	-30.373972	5.056319	4.631039
H	-31.355639	6.030148	3.503012
H	-32.136530	4.799013	4.505649

E = -10643.7192087 Hartree

P(NDI2OD-T2), n = 5, UωB97X-D/6-31G*, charged state

C	25.813369	0.250643	-0.858830
C	24.910526	-0.673899	-1.425397
C	23.573454	-0.385442	-1.492894
C	23.046483	0.843902	-1.034299
C	23.921297	1.787464	-0.512934
C	25.301077	1.483036	-0.398421
C	26.199347	2.401780	0.185068
C	27.522295	2.081956	0.325765
C	28.048134	0.847339	-0.121543
C	27.195254	-0.051833	-0.747879
C	23.460771	3.160554	-0.142990
N	24.386870	4.006044	0.478310
C	25.731058	3.720604	0.686028
C	27.702969	-1.306091	-1.386853
N	26.750381	-2.211775	-1.868750
C	25.379505	-1.988649	-1.934836
O	26.477986	4.503247	1.226025
O	22.347104	3.567532	-0.365123
O	28.874721	-1.560868	-1.517426
O	24.618267	-2.808447	-2.392964
C	23.882971	5.318753	0.876717
C	27.279318	-3.451937	-2.432407
H	22.898762	-1.129846	-1.898920
H	27.855383	-3.238814	-3.333553
H	27.936073	-3.931419	-1.708046
H	26.439876	-4.097036	-2.671161
H	24.688871	5.849879	1.372810
H	23.549736	5.871756	-0.001450
H	23.036111	5.198596	1.551642
H	28.177335	2.793553	0.814841
C	29.472315	0.590618	0.164861
C	30.007226	-0.340057	1.003782
C	31.416012	-0.241114	1.118196
C	31.948871	0.767639	0.363735
S	30.703962	1.602752	-0.508070
C	33.342803	1.161276	0.219854
C	33.862298	2.417381	0.065598
C	35.278999	2.426277	-0.044738
C	35.817014	1.178618	0.029883
S	34.605946	-0.029485	0.214769
H	29.405866	-1.071691	1.528211
H	32.016912	-0.877601	1.755834
H	33.248798	3.310123	0.057225
H	35.869822	3.325526	-0.163013
H	36.858735	0.897105	-0.017340
C	21.582454	1.005768	-1.138289
C	20.844658	1.055474	-2.283376
C	19.450140	1.157774	-2.041872
C	19.135735	1.156239	-0.711632
S	20.565119	1.017114	0.260208
C	17.825259	1.240504	-0.084697
C	17.479973	1.853866	1.086563
C	16.094593	1.753963	1.379370
C	15.400672	1.050109	0.442195
S	16.439691	0.511003	-0.830761
C	13.937454	0.839277	0.390344
C	13.296066	-0.372592	0.605040
C	11.887583	-0.457315	0.475313
C	11.116437	0.685852	0.172703
C	11.789967	1.911361	-0.011149
C	13.155357	1.974386	0.083256
C	11.217329	-1.688691	0.640635
C	9.862110	-1.766359	0.472642
C	9.075707	-0.631769	0.156119
C	9.704423	0.602746	0.049853
C	11.965083	-2.930742	0.967431
C	14.051542	-1.588695	1.035326
N	13.337211	-2.785556	1.145606
C	11.044759	3.155788	-0.333852
C	8.931423	1.876733	-0.091967
N	9.660906	3.043500	-0.358594
C	14.119171	-3.961566	1.521274
C	8.870739	4.255080	-0.567585
O	11.608615	4.205114	-0.543309
O	7.734013	1.949991	0.026062
O	15.230171	-1.577812	1.294285
O	11.414470	-4.000606	1.082593
H	9.385248	-2.735280	0.565220
H	13.646120	2.924578	-0.091098
H	18.191028	2.389718	1.703037
H	15.627147	2.182280	2.257189
H	21.291938	1.055583	-3.269680
H	18.706466	1.254532	-2.823021
H	9.548280	5.047509	-0.868892

H	8.124031	4.075393	-1.339562
H	8.355903	4.531575	0.353133
H	14.915632	-4.120565	0.794769
H	14.570379	-3.811236	2.501975
H	13.449257	-4.815135	1.541363
C	7.642291	-0.859684	-0.089909
C	6.936287	-0.623204	-1.232216
C	5.584533	-1.034346	-1.147141
C	5.264046	-1.584087	0.064388
S	6.640107	-1.590619	1.118151
C	3.977859	-2.085527	0.523885
C	3.712951	-3.173642	1.307205
C	2.328423	-3.347755	1.565559
C	1.549111	-2.407712	0.960025
S	2.513902	-1.255623	0.105031
H	7.377118	-0.169904	-2.110940
H	4.871840	-0.952583	-1.958175
H	4.484415	-3.843726	1.666423
H	1.917376	-4.157169	2.155784
C	0.085233	-2.244941	1.091273
C	-0.841290	-2.449383	0.075938
C	-2.212419	-2.195810	0.311043
C	-2.674148	-1.773171	1.577403
C	-1.716832	-1.618888	2.601346
C	-0.384673	-1.834040	2.354041
C	-3.165685	-2.354285	-0.720484
C	-4.476910	-2.049968	-0.501663
C	-4.961793	-1.585438	0.752945
C	-4.052403	-1.505217	1.810379
C	-2.114819	-1.206844	3.970242
C	-4.483157	-1.256590	3.218742
N	-3.476524	-1.063192	4.180892
C	-0.428241	-2.999032	-1.249899
C	-2.761771	-2.813538	-2.073847
N	-1.410560	-3.111419	-2.236519
O	0.700133	-3.354325	-1.495802
O	-3.553123	-2.933777	-2.979442
O	-1.302296	-1.030251	4.850968
O	-5.632940	-1.233275	3.581971
C	-0.959075	-3.620406	-3.528769
C	-3.940950	-0.763529	5.533044
H	0.323807	-1.672331	3.157875
H	-5.163120	-2.135894	-1.335932
H	-0.541451	-4.620044	-3.408843
H	-1.813926	-3.645539	-4.196834
H	-0.183379	-2.968709	-3.930868
H	-3.071448	-0.534195	6.140876
H	-4.624564	0.083820	5.507307
H	-4.472862	-1.621261	5.946014
C	-6.362414	-1.170625	0.792783
C	-6.905277	-0.029999	1.320743
C	-8.275602	0.130449	1.036180
C	-8.801976	-0.897649	0.290766
S	-7.584077	-2.081164	-0.051984
C	-10.159216	-1.081381	-0.175330
C	-10.593641	-1.758498	-1.286974
C	-11.994022	-1.714078	-1.456701
C	-12.637577	-1.007347	-0.479842
S	-11.507011	-0.396646	0.677418
H	-6.324212	0.690516	1.880534
H	-8.860431	0.988243	1.343120
H	-9.918180	-2.248164	-1.979274
H	-12.524300	-2.192103	-2.269319
C	-14.070374	-0.674715	-0.368090
C	-14.412510	0.665268	-0.401154
C	-15.741505	1.092850	-0.422124
C	-16.793273	0.153293	-0.443268
C	-16.454751	-1.236793	-0.381152
C	-15.103139	-1.650269	-0.313037
C	-17.507994	-2.174260	-0.377973
C	-18.833593	-1.749964	-0.492431
C	-19.171862	-0.412035	-0.579223
C	-18.144108	0.566005	-0.511279
C	-18.449151	1.997389	-0.426520
C	-16.011074	2.525116	-0.455106
C	-17.241696	-3.604792	-0.285166
C	-14.812112	-3.069926	-0.097639
N	-17.361027	2.882292	-0.449634
N	-15.898581	-3.956509	-0.140941
O	-13.701992	-3.527755	0.122770
O	-18.117485	-4.457170	-0.312927
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O	-19.572569	2.464265	-0.328896
H	-13.641249	1.425327	-0.450795
H	-19.602241	-2.512320	-0.546762
C	-15.571795	-5.363426	0.036474
C	-17.698237	4.297159	-0.402552
H	-15.116671	-5.523332	1.015268
H	-16.494037	-5.929710	-0.050467
H	-14.854457	-5.678667	-0.722378
H	-16.773597	4.860668	-0.481322
H	-18.372604	4.546859	-1.222437
H	-18.207180	4.531920	0.534031
C	-20.591558	-0.087795	-0.823124
C	-21.159677	0.483731	-1.924980
C	-22.568840	0.564540	-1.852034
C	-23.082017	0.050501	-0.689788
S	-21.802688	-0.524452	0.332265
C	-24.471606	-0.053179	-0.290558
C	-25.071393	-0.987126	0.515149
C	-26.456145	-0.761109	0.690762
C	-26.924614	0.319653	-0.006544
S	-25.627669	1.118931	-0.833351
H	-23.193643	0.956038	-2.646625
H	-20.570764	0.838822	-2.760317
H	-24.534094	-1.823092	0.944448
H	-27.100556	-1.400921	1.282425
C	-28.291872	0.851079	0.031350
C	-29.055731	1.217901	-1.074004
C	-30.307289	1.862668	-0.888961
C	-30.822895	2.059352	0.408557
C	-30.075694	1.608354	1.516892
C	-28.846089	1.042364	1.326805
H	-28.263855	0.753358	2.193970
C	-28.671266	0.841286	-2.465230
C	-31.062434	2.333610	-1.986151
C	-32.270724	2.963542	-1.790141
C	-32.782876	3.140777	-0.497671
C	-32.067223	2.692783	0.588402
C	-30.563586	2.166170	-3.375065
C	-30.598235	1.779326	2.898871
C	-32.613483	2.881684	1.956721
N	-31.840068	2.413153	3.018727
N	-29.389960	1.438090	-3.513652
O	-27.802413	0.047392	-2.726698
O	-31.157617	2.616597	-4.329645
O	-29.990664	1.394073	3.869659
O	-33.680375	3.413933	2.163351
C	-28.917314	1.132912	-4.861664
C	-32.395783	2.610930	4.354383
H	-33.736647	3.628492	-0.335989
H	-32.813596	3.318813	-2.657848
H	-29.076673	0.077541	-5.086859
H	-29.473866	1.750774	-5.559154
H	-27.850951	1.342267	-4.929704
H	-31.685455	2.220187	5.075904
H	-32.566732	3.673090	4.529119
H	-33.348847	2.088795	4.441849

E = -10643.8136191 Hartree