Supporting Information for

Polarons in π-conjugated ladder-type polymers: a broken symmetry density functional description.

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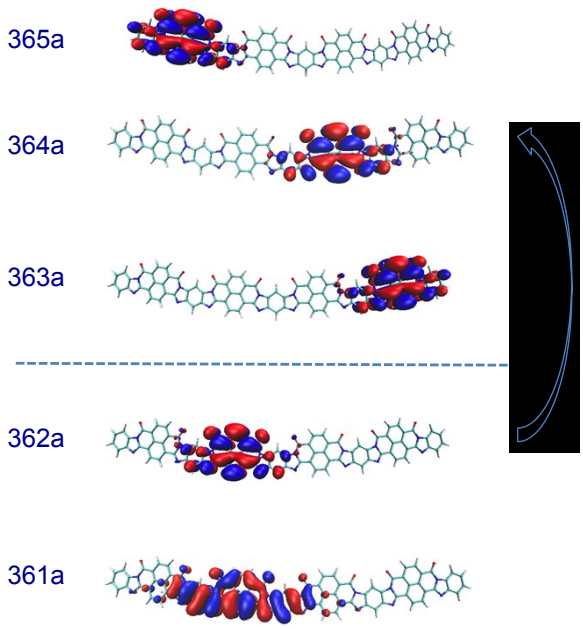
S1. Spin contamination values (ωB97X-D3/6-31G*) for *cis* and *trans* BBL oligomers (*n*), considering the single charged (polaron) and double charged (bipolaron) states.

<S2> polaron (-1)**				
	cis		*trans*	
n	UDFT	BS-UDFT	UDFT	BS-UDFT
1	0.7760		0.7777	
2	0.7814		0.8792	0.7840
3	0.7769		0.7831	
4	0.7804	0.7769	0.8780	0.7836
5	0.7643	0.7767	0.8704	0.7838
6	0.7623	0.7769	0.8700	0.7839
7	0.7597	0.7769	-	-
8	0.7623	0.7769	0.8699	0.7840

<S2> bipolaron (-2)**				
	cis		*trans*	
n	RDFT	BS-UDFT	RDFT	BSU-DFT
1	0.000		0.000	
2	0.000	1.0525	0.000	1.0562
3	0.000	1.0530	0.000	1.0598
4	0.000	1.0530	0.000	1.0623
5	0.000	1.0532	0.000	1.0731
6	0.000	1.0533	0.000	1.0668
7	-	-	-	-
8	0.000	1.0534	0.000	1.0638

S2. Calculation of the coupling integral H_{ab} and TD-BSUDFT value for the first dipole active excited state. MOs at the BS-UDFT geometries are also reported for BBL*4*. ωB97X-D3/6-31G* level has been adopted (BS-UDFT method).

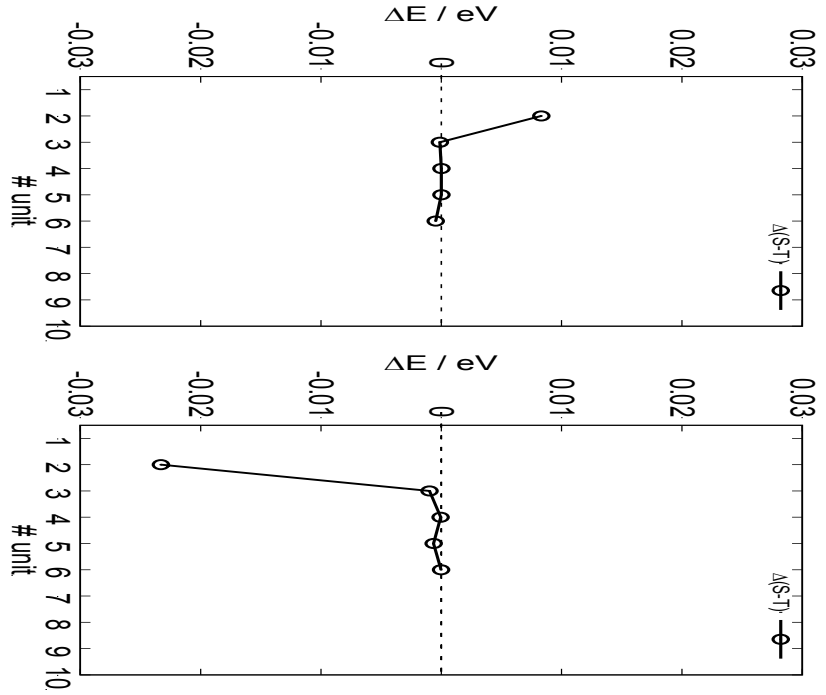


TD - BS-(U)DFT

S1 = 1.1476 eV f=0.0055

361A -> 364A	-0.15228
362A -> 363A	-0.14371
362A -> 364A	**0.94540**
362A -> 365A	0.10524
362A -> 371A	0.11748

S3. Computed energy difference between the singlet and the triplet state Δ(S-T) for a double charged state (bipolaron) for each length. ΔE = E(S) – E(T) computed at the BS-UDFT and UDFT levels (ωB97X-D3/6-31G*), respectively.



S4. First roots (S1 and S2) computed for BBL*5*, single charged state (polaron) at the TD-UDFT (negative value for S1) and TD-BS-UDFT (positive values) levels. Calculations are carried out at the ωB97X-D3/6-31G* level (UDFT and BS-UDFT methods).

TD – UDFT

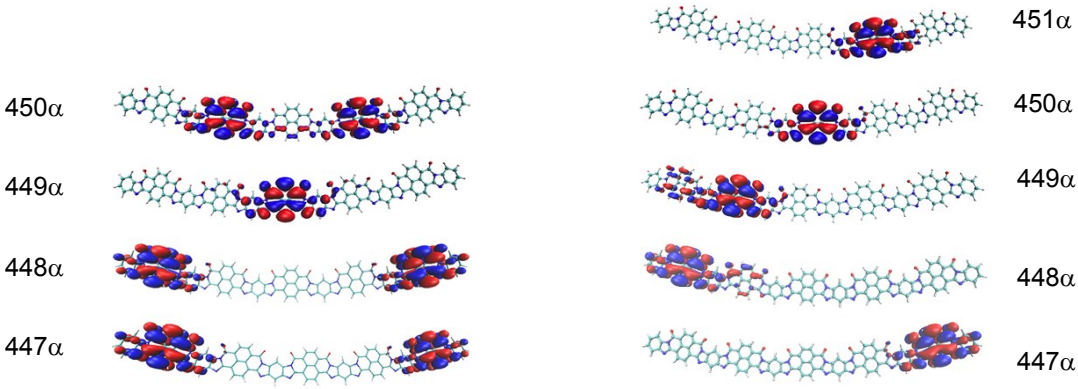
S1 = -0.0039 eV (-314752.04 nm) f=-0.0011
447A -> 448A 6.10318
447A <- 448A -6.02069

S2 = 0.4963 eV (2498.04 nm) f=0.0000
447A -> 449A -0.56694
447A -> 450A 0.81772

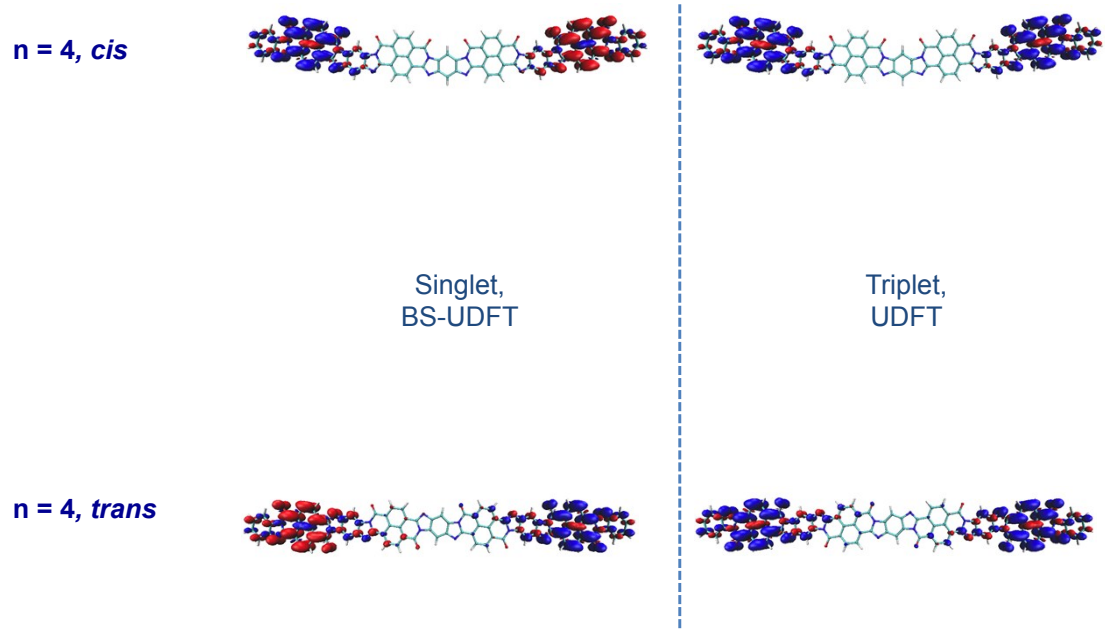
TD – BS-UDFT

S1 = 0.9812 eV 1263.60 nm f=0.0002
447A -> 448A 0.72458
447A -> 449A -0.64781
447A -> 450A 0.17236
447A -> 451A -0.15451

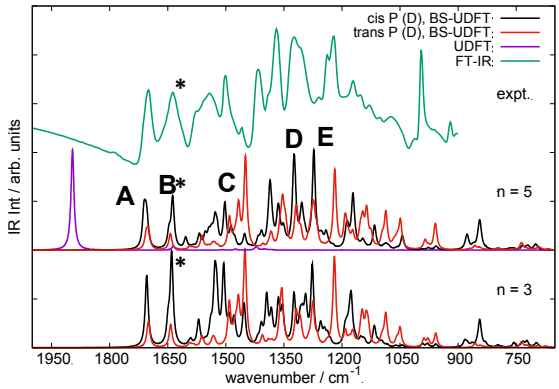
S2 = 1.0098 eV 1227.81 nm f=0.0053
446A -> 451A -0.13551
447A -> 448A 0.31779
447A -> 450A -0.26163
447A -> 451A 0.87952



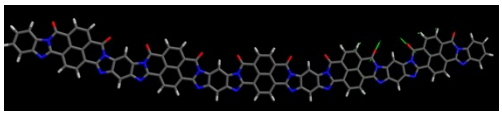
S5. Computed spin density for BBL*4*, double charged state (bipolaron) in its singlet (BS-UDFT scheme, biradicaloid character) and triplet (UDFT scheme) multiplicity. Calculations are carried out at the ωB97X-D3/6-31G* level (BS-UDFT method for bipolaron and UDFT for triplet state).



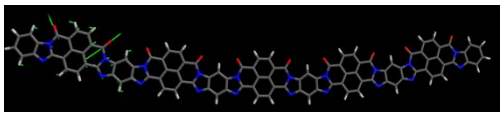
S6. Computed IR spectra for BBL*3* and BBL*5* in the charged (polaron) state, compared with the IR spectrum of TDAE-doped BBL film (as reported in the manuscript). Normal modes for the main IR active bands (labelled as: A, B, C, D, E) are reported. Calculations are carried out at the ωB97X-D3/6-31G* level (UDFT and BS-UDFT methods for the polaron state).



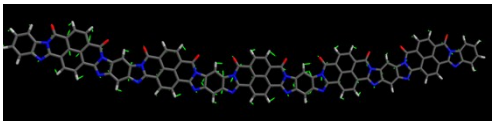
Mode A: C=O symmetric stretching



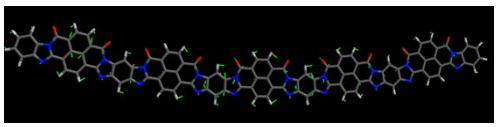
Mode B (*): C=O anti-symmetric stretching



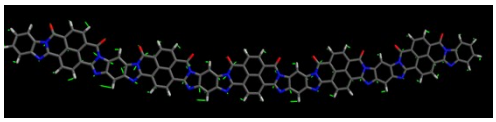
Mode C: C=C/C-C stretching/shrinking on napthalene core



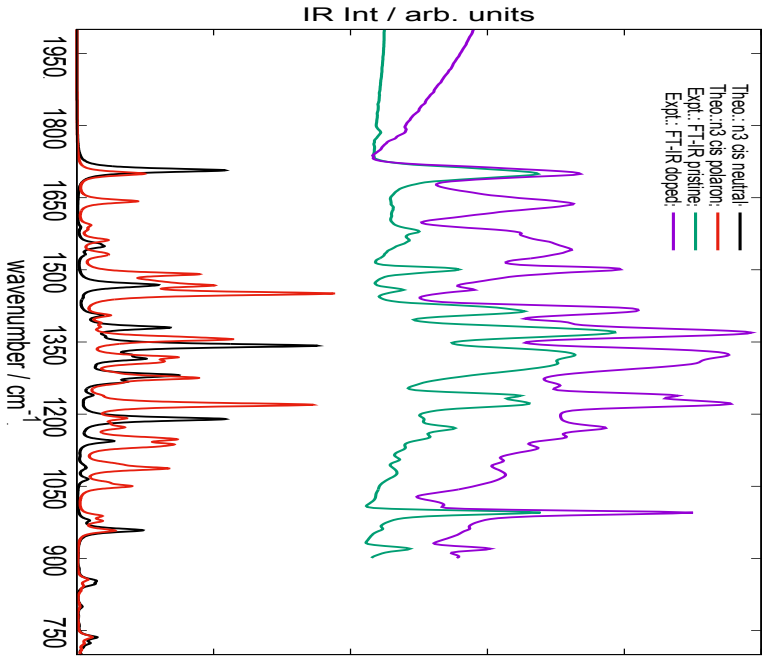
Mode D: C=C/C-C stretching/shrinking on central unit



Mode E: CN stretching + CH bending



S7. Computed IR spectra for BBL*3* in the neutral (black) and charged (polaron) state (red), compared with the IR spectrum of pristine (green) and TDAE-doped BBL (purple) film. Calculations are carried out at the ωB97X-D3/6-31G* level (unrestricted method for the polaron state). The label * indicates the main IR active polaron band.



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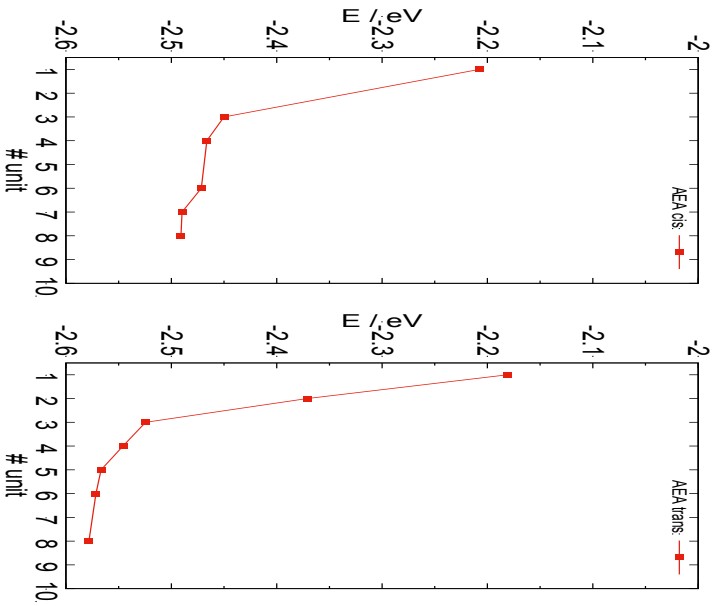

S8. Calculated Adiabatic Electron Affinities (AEA) *vs.* oligomer length

S9. BBL*4 cis* neutral and charged (-1) states computed with augmented basis set (6-31++G*) and w-B97XD functional.

6-31G* calculations

E(neutral, 6-31G*, DFT) = -4771.93058488 Hartree
E(-1, 6-31G*, UDFT) = -4772.01136729 Hartree
E(-1, 6-31G*, BS-UDFT) = -4772.02121893 Hartree

ΔE(E(BS-UDFT) – E(UDFT)) = **-0.27 eV**

E(-2, 6-31G*, DFT) = -4772.01636514 Hartree
E(-2, 6-31G*, BS-UDFT) = -4772.08569769 Hartree

ΔE(E(BS-UDFT) – E(DFT)) = **-1.88 eV**

6-31++G* calculations

E(-1, 6-31++G*, UDFT) = -4772.12729671 Hartree
E(-1, 6-31++G*, BS-UDFT, *single point*) = -4772.13131851 Hartree

ΔE(E(BS-UDFT) – E(UDFT)) = **-0.11 eV**

E(-2, 6-31++G*, DFT) = -4772.13993874 Hartree
E(-2, 6-31++G*, BS-UDFT, *single point*) = -4772.20414753 Hartree

ΔE(E(BS-UDFT) – E(DFT)) = **-1.74 eV**

S10. B3LYP calculations for BBL*4* and BBL6 *cis*

BBL*4*
B3LYP/6-31G* calculations

Neutral state E(B3LYP) = -4773.48840419 Hartree

Charged (-1) state E(UB3LYP) = -4773.59554361 Hartree
No BS for the -1 charged state.

Charged (-2) state E(B3LYP) = -4773.64339058 Hartree
Charged (-2) state E(BS-UB3LYP, *single point*) = -4773.81180223 Hartree

BBL*6*
B3LYP/6-31G* calculations

Neutral state E(B3LYP) = -7044.10875385 Hartree

Charged (-1) state E(UB3LYP) = -7044.23579545 Hartree
No BS for the -1 charged state.

Charged (-2) state E(B3LYP) = -7044.30990340 Hartree
Charged (-2) state E(BS-UB3LYP, *single point*) = -7044.31691793 Hartree

S11. B2PLYP calculations for BBL*2 trans*

We considered *BBL2 trans* as a case study, in the neutral, charged (-1 and -2) states. For the -1 charged state we did not find any wavefunction instability at the B2PLYP level (to note, the *trans* species does already show an instability for the polaron and the bipolaron at the w-B97XD level, see **Figure 1** of the manuscript). For the -2 charged state, similarly to B3LYP, we did find a wavefunction instability at the B2PLYP level. A closer look to the bond length differences between the -1 charged and the neutral states (here reported in **Figure R1**), reveals that B2PLYP tend to delocalize the charge with very low bond length distortion values, similarly to the case of B3LYP.

Charged (-1) state E(UB2PLYP) = -2497.87365796 Hartree
No BS for the -1 charged state.

Charged (-2) state E(B2PLYP) = -2497.85752478 Hartree
Charged (-2) state E(BS-UB2PLYP): an internal instability in the wavefunction has been found, however - for the porpuses of this work - the state has not been further re-optimized.

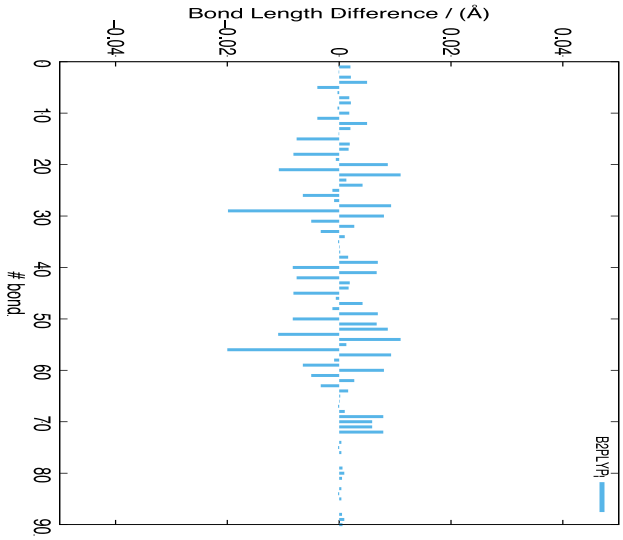
Bond Length Difference / (Å)
−0.04
−0.02
0
0.02
0.04
0
10
20
30
40
50
60
70
80
90
bond
B2PLYP

Figure R1

S12. **Optimized Geometries**
All optimized geometries, for each *cis* and *trans* BBL conformer, are available under request to the corresponding author (dfazzi@uni-koeln.de).
Here below, we report the representative case for BBL*4 cis*.

BBL4 *cis*

Neutral state (charge 0, spin multeplicity 1) – wB97XD/6-31G*

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

Charged state (charge -1, spin multeplicity 2) UwB97XD/6-31G*

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

Charged state (charge -1, spin multeplicity 2) Broken Symmetry, BS-UwB97XD/6-31G*

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
N	9.785491	-2.678081	-0.054818
C	11.900323	0.269779	0.218929
C	13.142571	-0.318931	0.023516
C	13.342958	-1.703349	-0.200745
C	12.275411	-2.592980	-0.240674
N	14.696301	-1.981408	-0.369114
C	15.300322	-0.839911	-0.257829
N	14.429021	0.229016	-0.015251
C	16.727137	-0.586405	-0.364430
C	17.174860	0.752633	-0.211602
C	16.265557	1.814309	0.039166
C	14.799038	1.562019	0.148819
C	18.555750	1.035614	-0.313365
C	19.463904	-0.025338	-0.568304
C	19.002347	-1.318064	-0.712478
C	17.631643	-1.599433	-0.609707
C	19.000940	2.375967	-0.158933
C	20.446748	2.719279	-0.257877
N	21.283044	1.631338	-0.513276
C	20.875602	0.301883	-0.672402
C	22.671991	1.628868	-0.667158
C	22.998370	0.283979	-0.910522
N	21.858891	-0.513050	-0.906403
C	23.628661	2.636968	-0.618491
C	24.946164	2.246248	-0.826867
C	25.290686	0.907198	-1.072336
C	24.326226	-0.088815	-1.117371
C	16.723452	3.105067	0.184682
C	18.097253	3.386616	0.085768
C	5.130699	1.581498	0.877646
C	6.530967	1.683634	0.817432
O	20.885243	3.843106	-0.132214
O	13.983778	2.433604	0.360892
O	9.362475	1.775512	0.656540
O	2.333045	1.283727	0.962390
N	-2.490384	-3.235119	0.218592
C	-3.253566	-2.174563	0.370417
N	-2.525972	-1.000804	0.578419
C	-3.065914	0.291721	0.764367
C	-4.514613	0.343317	0.712928
C	-5.286392	-0.831631	0.494989
C	-4.685878	-2.102945	0.328617
C	-6.710778	-0.728478	0.434601

C	-7.470879	-1.901843	0.211409
C	-6.843492	-3.149865	0.055704
C	-5.470622	-3.249300	0.113191
C	-7.322569	0.545877	0.593274
C	-6.526022	1.687437	0.815051
C	-5.155471	1.588268	0.873784
C	-8.763522	0.702178	0.524216
N	-9.465445	-0.501646	0.290833
C	-8.897503	-1.768242	0.138575
N	-9.788895	-2.712403	-0.069939
C	-11.005435	-2.064357	-0.064402
C	-10.837555	-0.667119	0.160449
C	-12.273581	-2.607870	-0.251475
C	-13.334694	-1.710741	-0.208226
C	-13.127397	-0.327470	0.017810
C	-11.880818	0.250677	0.211832
N	-14.415637	0.228752	-0.018372
C	-15.291399	-0.837705	-0.261133
N	-14.691038	-1.980754	-0.374781
C	-14.784095	1.555578	0.146228
C	-16.254850	1.810325	0.037886
C	-17.167559	0.752562	-0.212381
C	-16.717346	-0.586272	-0.366337
C	-18.548502	1.036994	-0.312329
C	-19.457133	-0.022943	-0.566714
C	-18.993749	-1.315841	-0.712000
C	-17.624012	-1.598728	-0.611297
C	-18.990687	2.378405	-0.156300
C	-18.082517	3.386209	0.088055
C	-16.709590	3.101937	0.185039
C	-20.433080	2.723192	-0.253170
N	-21.272184	1.635125	-0.508410
C	-20.867832	0.304530	-0.668892
N	-21.855128	-0.507827	-0.901992
C	-22.991401	0.292846	-0.903672
C	-22.660778	1.636925	-0.659996
C	-24.321104	-0.074487	-1.108493
C	-25.283025	0.924346	-1.061384
C	-24.934308	2.262006	-0.815709
C	-23.614733	2.647515	-0.609276
O	-2.316055	1.245183	0.943812
O	-9.380541	1.754706	0.645341
O	-13.977974	2.436795	0.358854
O	-20.875596	3.846526	-0.127147
H	-19.708494	-2.108595	-0.906469
H	-17.255694	-2.612425	-0.726471
H	-18.448369	4.400946	0.203855
H	-15.987679	3.888781	0.375356
H	-23.335224	3.675350	-0.419612
H	-25.713707	3.017150	-0.786208
H	-26.327053	0.670362	-1.218011
H	-24.577297	-1.111512	-1.297154
H	-7.464999	-4.022687	-0.114081
H	-4.969179	-4.203316	-0.010289
H	-7.026564	2.642331	0.934268
H	-4.535049	2.462197	1.040950
H	-11.722191	1.304559	0.382415
H	-12.423549	-3.666618	-0.425921
H	4.948356	-4.163902	0.005984
H	7.448870	-3.988384	-0.097395
H	4.513115	2.457630	1.042816

H	7.022665	2.643399	0.935322
H	-0.054019	0.472575	0.843145
H	0.005081	-4.546741	0.029935
H	17.263886	-2.613525	-0.723976
H	19.716652	-2.110874	-0.907290
H	16.005467	3.895451	0.375359
H	18.465777	4.400399	0.200307
H	11.757854	1.326561	0.386933
H	12.415144	-3.653110	-0.413550
H	24.578867	-1.126630	-1.305773
H	26.333622	0.650463	-1.230325
H	25.728083	2.998643	-0.799167
H	23.354243	3.666201	-0.429135

Charged state (charge -2, spin multeplicity 1) wB97XD/6-31G*

C	0.000001	-0.526117	0.000552
C	-1.159072	-1.291498	0.000436
C	-1.180301	-2.710228	0.000231
C	0.000000	-3.446732	0.000135
C	1.180302	-2.710229	0.000231
C	1.159074	-1.291499	0.000436
N	-2.486207	-3.180876	0.000127
C	-3.239438	-2.117525	0.000281
N	-2.506579	-0.923829	0.000491
C	-4.683138	-2.056662	0.000249
C	-5.293882	-0.774618	0.000370
C	-4.523138	0.417367	0.000564
C	-3.041446	0.366845	0.000677
C	-6.708664	-0.680482	0.000300
C	-7.486003	-1.870182	0.000125
C	-6.860244	-3.109747	0.000024
C	-5.468211	-3.201984	0.000081
C	-7.316094	0.601395	0.000411
C	-8.795352	0.746414	0.000321
N	-9.495069	-0.459537	0.000143
C	-8.924651	-1.738513	0.000066
C	-10.880966	-0.649397	0.000088
C	-11.045521	-2.058651	-0.000046
N	-9.810026	-2.694031	-0.000064
C	-11.930874	0.259836	0.000116
C	-13.180443	-0.347344	-0.000002
C	-13.390079	-1.754792	-0.000139
C	-12.310908	-2.636204	-0.000158
N	-14.739033	-2.049561	-0.000251
C	-15.349406	-0.887345	-0.000178
N	-14.463755	0.194795	-0.000043
C	-16.761093	-0.631472	-0.000256
C	-17.190433	0.722558	-0.000160
C	-16.265899	1.798837	0.000016
C	-14.819716	1.553034	0.000117
C	-18.587870	1.006998	-0.000244
C	-19.510298	-0.070246	-0.000413
C	-19.054143	-1.394302	-0.000498
C	-17.699014	-1.671686	-0.000423
C	-19.017294	2.361637	-0.000151
C	-20.440645	2.702285	-0.000236
N	-21.299158	1.592537	-0.000416
C	-20.910935	0.248546	-0.000490
C	-22.692611	1.593713	-0.000511

C	-23.048848	0.230001	-0.000627
N	-21.930266	-0.580089	-0.000615
C	-23.634322	2.617228	-0.000506
C	-24.971677	2.235191	-0.000617
C	-25.347554	0.882003	-0.000732
C	-24.399330	-0.131081	-0.000740
C	-16.721282	3.121615	0.000106
C	-18.077587	3.398573	0.000022
C	-5.143802	1.654665	0.000670
C	-6.539495	1.746655	0.000592
O	-20.893974	3.839651	-0.000173
O	-13.962885	2.423916	0.000265
O	-9.366730	1.819154	0.000533
O	-2.326339	1.350337	0.000840
N	2.486207	-3.180878	0.000126
C	3.239439	-2.117527	0.000281
N	2.506580	-0.923831	0.000490
C	3.041447	0.366844	0.000676
C	4.523139	0.417365	0.000563
C	5.293882	-0.774620	0.000369
C	4.683138	-2.056664	0.000248
C	6.708665	-0.680483	0.000299
C	7.486003	-1.870183	0.000124
C	6.860243	-3.109749	0.000023
C	5.468211	-3.201986	0.000080
C	7.316094	0.601394	0.000409
C	6.539495	1.746654	0.000591
C	5.143803	1.654665	0.000669
C	8.795352	0.746413	0.000320
N	9.495069	-0.459539	0.000142
C	8.924651	-1.738515	0.000065
N	9.810026	-2.694034	-0.000065
C	11.045521	-2.058653	-0.000046
C	10.880965	-0.649399	0.000087
C	12.310908	-2.636206	-0.000159
C	13.390079	-1.754793	-0.000140
C	13.180442	-0.347346	-0.000002
C	11.930873	0.259835	0.000116
N	14.463754	0.194794	-0.000044
C	15.349406	-0.887345	-0.000178
N	14.739034	-2.049562	-0.000252
C	14.819715	1.553033	0.000117
C	16.265898	1.798837	0.000016
C	17.190433	0.722558	-0.000160
C	16.761093	-0.631472	-0.000256
C	18.587869	1.006999	-0.000244
C	19.510298	-0.070245	-0.000412
C	19.054143	-1.394302	-0.000498
C	17.699014	-1.671685	-0.000422
C	19.017293	2.361638	-0.000151
C	18.077587	3.398573	0.000021
C	16.721281	3.121614	0.000106
C	20.440644	2.702286	-0.000236
N	21.299158	1.592539	-0.000416
C	20.910935	0.248547	-0.000489
N	21.930266	-0.580088	-0.000614
C	23.048848	0.230002	-0.000626
C	22.692611	1.593715	-0.000510
C	24.399330	-0.131080	-0.000739
C	25.347553	0.882005	-0.000731
C	24.971676	2.235193	-0.000615

C	23.634321	2.617229	-0.000505
O	2.326339	1.350336	0.000840
O	9.366731	1.819152	0.000533
O	13.962884	2.423915	0.000264
O	20.893972	3.839652	-0.000173
H	19.788240	-2.193218	-0.000622
H	17.336001	-2.693935	-0.000493
H	18.441742	4.420310	0.000084
H	15.984780	3.917867	0.000244
H	23.324773	3.654013	-0.000414
H	25.740965	3.002185	-0.000611
H	26.403629	0.625354	-0.000817
H	24.681240	-1.179168	-0.000831
H	7.476448	-4.002478	-0.000105
H	4.976528	-4.169060	-0.000009
H	7.036447	2.710729	0.000671
H	4.525270	2.545689	0.000824
H	11.795308	1.330517	0.000234
H	12.449968	-3.710682	-0.000269
H	-4.976528	-4.169058	-0.000008
H	-7.476448	-4.002476	-0.000104
H	-4.525269	2.545689	0.000825
H	-7.036447	2.710730	0.000672
H	0.000002	0.553212	0.000735
H	-0.000000	-4.530086	-0.000027
H	-17.336000	-2.693935	-0.000493
H	-19.788240	-2.193219	-0.000623
H	-15.984782	3.917867	0.000245
H	-18.441743	4.420310	0.000084
H	-11.795310	1.330519	0.000235
H	-12.449967	-3.710681	-0.000268
H	-24.681240	-1.179170	-0.000833
H	-26.403629	0.625352	-0.000818
H	-25.740966	3.002183	-0.000612
H	-23.324774	3.654012	-0.000414

Charged state (charge -2, spin multeplicity 1) Broken Symmetry, BS-UwB97XD/6-31G*

C	0.000000	-0.419523	-0.000055
C	-1.158717	-1.185711	-0.000040
C	-1.177463	-2.602986	-0.000016
C	0.000000	-3.341117	-0.000005
C	1.177463	-2.602986	-0.000016
C	1.158717	-1.185711	-0.000039
N	-2.485147	-3.077131	-0.000016
C	-3.236119	-2.018747	-0.000015
N	-2.508207	-0.822003	-0.000055
C	-4.687363	-1.965684	0.000010
C	-5.302968	-0.687039	0.000034
C	-4.536562	0.509078	0.000004
C	-3.049646	0.465640	-0.000099
C	-6.713832	-0.600437	0.000093
C	-7.486384	-1.792504	0.000100
C	-6.861115	-3.023900	0.000064
C	-5.461199	-3.109537	0.000028
C	-7.332735	0.676999	0.000138
C	-8.822556	0.815468	0.000248
N	-9.513813	-0.387512	0.000165
C	-8.932659	-1.662686	0.000113

C	-10.902575	-0.593732	0.000115
C	-11.048814	-2.002938	0.000075
N	-9.801870	-2.624180	0.000086
C	-11.966640	0.297630	0.000114
C	-13.208184	-0.329041	0.000064
C	-13.395496	-1.741848	0.000023
C	-12.302156	-2.604109	0.000030
N	-14.736192	-2.061777	-0.000022
C	-15.363517	-0.905667	-0.000006
N	-14.496617	0.188928	0.000043
C	-16.778779	-0.669523	-0.000037
C	-17.221914	0.674791	-0.000010
C	-16.310206	1.767303	0.000043
C	-14.876434	1.550397	0.000069
C	-18.627080	0.937348	-0.000039
C	-19.526662	-0.155171	-0.000093
C	-19.053354	-1.478046	-0.000118
C	-17.698885	-1.731931	-0.000091
C	-19.082762	2.285735	-0.000012
C	-20.499508	2.600942	-0.000039
N	-21.343941	1.471428	-0.000093
C	-20.933307	0.138135	-0.000120
C	-22.734844	1.449047	-0.000129
C	-23.068904	0.079101	-0.000174
N	-21.937727	-0.711814	-0.000169
C	-23.694896	2.457001	-0.000126
C	-25.025096	2.053580	-0.000170
C	-25.379023	0.693768	-0.000216
C	-24.414214	-0.303132	-0.000218
C	-16.798112	3.090361	0.000069
C	-18.150013	3.342670	0.000043
C	-5.163081	1.736626	0.000046
C	-6.566279	1.821190	0.000109
O	-20.984787	3.728668	-0.000016
O	-14.014456	2.423410	0.000121
O	-9.384062	1.891109	0.000119
O	-2.342011	1.451286	0.000007
N	2.485147	-3.077131	-0.000015
C	3.236119	-2.018747	-0.000014
N	2.508207	-0.822003	-0.000054
C	3.049646	0.465640	-0.000098
C	4.536562	0.509078	0.000005
C	5.302968	-0.687039	0.000036
C	4.687363	-1.965684	0.000011
C	6.713832	-0.600437	0.000095
C	7.486384	-1.792504	0.000102
C	6.861115	-3.023900	0.000066
C	5.461199	-3.109537	0.000029
C	7.332735	0.676999	0.000140
C	6.566279	1.821190	0.000111
C	5.163081	1.736626	0.000048
C	8.822556	0.815468	0.000251
N	9.513813	-0.387512	0.000168
C	8.932659	-1.662686	0.000115
N	9.801870	-2.624180	0.000088
C	11.048814	-2.002938	0.000077
C	10.902575	-0.593732	0.000117
C	12.302156	-2.604109	0.000031
C	13.395496	-1.741848	0.000024
C	13.208184	-0.329041	0.000065
C	11.966640	0.297630	0.000116

N	14.496617	0.188928	0.000044
C	15.363517	-0.905667	-0.000006
N	14.736192	-2.061777	-0.000022
C	14.876434	1.550397	0.000071
C	16.310206	1.767304	0.000044
C	17.221914	0.674791	-0.000010
C	16.778779	-0.669523	-0.000037
C	18.627080	0.937348	-0.000039
C	19.526662	-0.155171	-0.000094
C	19.053354	-1.478046	-0.000119
C	17.698885	-1.731931	-0.000091
C	19.082762	2.285735	-0.000012
C	18.150013	3.342670	0.000043
C	16.798112	3.090361	0.000070
C	20.499508	2.600942	-0.000040
N	21.343941	1.471428	-0.000094
C	20.933307	0.138135	-0.000122
N	21.937727	-0.711814	-0.000170
C	23.068904	0.079101	-0.000176
C	22.734844	1.449047	-0.000131
C	24.414214	-0.303132	-0.000221
C	25.379023	0.693768	-0.000218
C	25.025096	2.053580	-0.000172
C	23.694896	2.457001	-0.000128
O	2.342011	1.451286	0.000007
O	9.384062	1.891109	0.000121
O	14.014456	2.423410	0.000122
O	20.984787	3.728668	-0.000016
H	19.778311	-2.285198	-0.000161
H	17.315484	-2.746845	-0.000110
H	18.532552	4.357799	0.000063
H	16.074676	3.898750	0.000111
H	23.400223	3.498116	-0.000092
H	25.807157	2.807871	-0.000172
H	26.430964	0.419725	-0.000253
H	24.679161	-1.355845	-0.000257
H	7.472126	-3.920052	0.000070
H	4.967171	-4.075465	0.000009
H	7.067260	2.783201	0.000150
H	4.553094	2.633703	0.000022
H	11.856923	1.371380	0.000152
H	12.421993	-3.681009	-0.000001
H	-4.967171	-4.075465	0.000007
H	-7.472126	-3.920052	0.000068
H	-4.553094	2.633703	0.000021
H	-7.067260	2.783201	0.000148
H	0.000000	0.660008	-0.000082
H	0.000000	-4.424396	0.000009
H	-17.315484	-2.746845	-0.000109
H	-19.778311	-2.285198	-0.000160
H	-16.074676	3.898750	0.000110
H	-18.532552	4.357799	0.000062
H	-11.856923	1.371380	0.000150
H	-12.421993	-3.681009	-0.000002
H	-24.679161	-1.355845	-0.000254
H	-26.430964	0.419725	-0.000250
H	-25.807157	2.807871	-0.000169
H	-23.400223	3.498116	-0.000091

Charged state (charge -2, spin multeplicity 3) UwB97XD/6-31G*

C	0.000000	0.418882	-0.000311
C	-1.158711	1.185080	-0.000245
C	-1.177461	2.602372	-0.000136
C	0.000000	3.340509	-0.000082
C	1.177461	2.602372	-0.000135
C	1.158711	1.185080	-0.000243
N	-2.485122	3.076491	-0.000105
C	-3.236106	2.018129	-0.000151
N	-2.508201	0.821388	-0.000295
C	-4.687360	1.965110	-0.000087
C	-5.303008	0.686512	-0.000081
C	-4.536654	-0.509622	-0.000206
C	-3.049726	-0.466224	-0.000443
C	-6.713868	0.599952	0.000060
C	-7.486383	1.792023	0.000140
C	-6.861059	3.023389	0.000107
C	-5.461175	3.108981	0.000013
C	-7.332806	-0.677461	0.000113
C	-8.822624	-0.815876	0.000369
N	-9.513888	0.387120	0.000270
C	-8.932670	1.662244	0.000191
C	-10.902627	0.593409	0.000195
C	-11.048779	2.002645	0.000164
N	-9.801833	2.623764	0.000185
C	-11.966803	-0.297832	0.000186
C	-13.208271	0.328991	0.000133
C	-13.395475	1.741809	0.000099
C	-12.302084	2.603944	0.000118
N	-14.736131	2.061939	0.000052
C	-15.363534	0.905847	0.000060
N	-14.496760	-0.188854	0.000105
C	-16.778792	0.669849	0.000026
C	-17.222033	-0.674452	0.000044
C	-16.310415	-1.767052	0.000091
C	-14.876644	-1.550314	0.000118
C	-18.627228	-0.936901	0.000015
C	-19.526747	0.155704	-0.000032
C	-19.053315	1.478526	-0.000049
C	-17.698826	1.732303	-0.000020
C	-19.083032	-2.285263	0.000034
C	-20.499781	-2.600373	0.000004
N	-21.344107	-1.470762	-0.000040
C	-20.933394	-0.137498	-0.000060
C	-22.735015	-1.448276	-0.000075
C	-23.068965	-0.078304	-0.000112
N	-21.937739	0.712555	-0.000103
C	-23.695160	-2.456149	-0.000075
C	-25.025327	-2.052617	-0.000115
C	-25.379133	-0.692775	-0.000153
C	-24.414233	0.304038	-0.000151
C	-16.798441	-3.090066	0.000109
C	-18.150367	-3.342263	0.000081
C	-5.163195	-1.737165	-0.000158
C	-6.566379	-1.821683	-0.000005
O	-20.985161	-3.728051	0.000020
O	-14.014714	-2.423369	0.000169
O	-9.384175	-1.891478	0.000048
O	-2.342124	-1.451886	-0.000250
N	2.485122	3.076491	-0.000101

C	3.236106	2.018129	-0.000147
N	2.508201	0.821388	-0.000292
C	3.049726	-0.466224	-0.000440
C	4.536654	-0.509622	-0.000202
C	5.303008	0.686512	-0.000075
C	4.687360	1.965110	-0.000081
C	6.713868	0.599952	0.000066
C	7.486383	1.792023	0.000147
C	6.861059	3.023389	0.000116
C	5.461175	3.108981	0.000020
C	7.332806	-0.677461	0.000119
C	6.566379	-1.821683	-0.000001
C	5.163195	-1.737165	-0.000154
C	8.822624	-0.815876	0.000376
N	9.513888	0.387120	0.000278
C	8.932670	1.662244	0.000199
N	9.801833	2.623764	0.000195
C	11.048779	2.002645	0.000173
C	10.902627	0.593409	0.000202
C	12.302084	2.603944	0.000128
C	13.395475	1.741809	0.000107
C	13.208271	0.328991	0.000138
C	11.966803	-0.297832	0.000191
N	14.496760	-0.188854	0.000110
C	15.363534	0.905847	0.000066
N	14.736131	2.061940	0.000060
C	14.876644	-1.550314	0.000122
C	16.310415	-1.767053	0.000092
C	17.222033	-0.674452	0.000046
C	16.778792	0.669849	0.000031
C	18.627228	-0.936901	0.000014
C	19.526747	0.155704	-0.000032
C	19.053315	1.478526	-0.000046
C	17.698826	1.732303	-0.000015
C	19.083032	-2.285263	0.000030
C	18.150368	-3.342263	0.000077
C	16.798441	-3.090066	0.000107
C	20.499781	-2.600374	-0.000002
N	21.344107	-1.470762	-0.000044
C	20.933394	-0.137498	-0.000061
N	21.937739	0.712555	-0.000102
C	23.068965	-0.078304	-0.000114
C	22.735015	-1.448276	-0.000080
C	24.414233	0.304038	-0.000154
C	25.379132	-0.692775	-0.000159
C	25.025327	-2.052617	-0.000124
C	23.695160	-2.456149	-0.000084
O	2.342124	-1.451886	-0.000249
O	9.384175	-1.891478	0.000052
O	14.014714	-2.423369	0.000170
O	20.985161	-3.728052	0.000013
H	19.778132	2.285793	-0.000080
H	17.315448	2.747221	-0.000025
H	18.532915	-4.357382	0.000088
H	16.075163	-3.898581	0.000143
H	23.400588	-3.497289	-0.000057
H	25.807456	-2.806838	-0.000129
H	26.431052	-0.418642	-0.000189
H	24.679081	1.356778	-0.000181
H	7.472101	3.919536	0.000173
H	4.967075	4.074886	0.000014

H	7.067474	-2.783641	0.000050
H	4.553155	-2.634214	-0.000255
H	11.857144	-1.371581	0.000226
H	12.421872	3.680854	0.000105
H	-4.967075	4.074886	0.000006
H	-7.472101	3.919536	0.000164
H	-4.553155	-2.634214	-0.000257
H	-7.067474	-2.783641	0.000046
H	0.000000	-0.660650	-0.000412
H	0.000000	4.423791	-0.000003
H	-17.315448	2.747221	-0.000032
H	-19.778132	2.285793	-0.000084
H	-16.075163	-3.898581	0.000144
H	-18.532915	-4.357382	0.000094
H	-11.857144	-1.371581	0.000222
H	-12.421872	3.680854	0.000095
H	-24.679081	1.356778	-0.000180
H	-26.431052	-0.418642	-0.000184
H	-25.807456	-2.806838	-0.000117
H	-23.400588	-3.497289	-0.000046