

Excited electronic states' properties of guanine quartet complexes with alkali metal cations

BRANISLAV Ž. MILOVANOVIĆ, MILENA M. PETKOVIĆ and MIHAJLO R. ETINSKI*

University of Belgrade - Faculty of Physical Chemistry, Studentski trg 12-16, 11 158

Belgrade, Serbia

Supplementary Material

Table S1. The Cartesian coordinates of the optimized geometry in Å of the G_4 system at M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure equals to -2169.646522 *a.u.*

Table S2. The Cartesian coordinates of the optimized geometry in Å of the $G_4\text{-Li}^+$ system at M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure equals to -2177.126452 *a.u.*

Table S3. The Cartesian coordinates of the optimized geometry in Å of the $G_4\text{-Na}^+$ system at M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure equals to -2331.854385 *a.u.*

Table S4. The Cartesian coordinates of the optimized geometry in Å of the $G_4\text{-K}^+$ system at M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure equals to -2769.46756 *a.u.*

Table S5. The Cartesian coordinates of the S_1 optimized geometry in Å of the G_4 system at CAM-B3LYP/6-31G level of theory. Energy of the optimized structure equals to -2167.995764 *a.u.*

Table S6. The Cartesian coordinates of the S_1 optimized geometry in Å of the $G_4\text{-Li}^+$ system at CAM-B3LYP/6-31G level of theory. Energy of the optimized structure equals to -2175.495151 *a.u.*

Table S7. The Cartesian coordinates of the S_1 optimized geometry in Å of the $G_4\text{-Na}^+$ system at CAM-B3LYP/6-31G level of theory. Energy of the optimized structure equals to -2330.408807 *a.u.*

Table S8. The Cartesian coordinates of the S_1 optimized geometry in Å of the $G_4\text{-K}^+$ system at CAM-B3LYP/6-31G level of theory. Energy of the optimized structure equals to -2767.870073 *a.u.*

*Corresponding author. E-mail: etinski@ffh.bg.ac.rs

Table S1. The Cartesian coordinates of the optimized geometry in Å of the G₄ system at M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure equals to -2169.646522 *a.u.*

N	4.912917	-1.627813	0.008094
O	2.133278	2.031048	0.001384
N	3.581953	0.260928	0.004161
C	4.847017	-0.289466	0.004061
N	5.956331	0.430482	0.000498
C	5.712325	1.754117	-0.002984
C	4.489107	2.410736	-0.003125
C	3.298803	1.624321	0.000764
N	6.639811	2.759799	-0.007223
C	5.943150	3.952567	-0.009712
N	4.650610	3.781201	-0.007330
H	4.079938	-2.207575	0.009577
H	5.822704	-2.057433	0.007095
H	2.782192	-0.376716	0.006288
H	7.640870	2.633743	-0.008343
H	6.452040	4.905834	-0.013200
N	-1.627761	-4.912391	-0.008887
O	2.031202	-2.132806	0.007465
N	0.260961	-3.581391	-0.000751
C	-0.289423	-4.846473	-0.004525
N	0.430521	-5.955797	-0.003626
C	1.754152	-5.711821	0.001197
C	2.410760	-4.488612	0.005165
C	1.624366	-3.298284	0.004300
N	2.759836	-6.639313	0.003108
C	3.952600	-5.942660	0.007991
N	3.781223	-4.650118	0.009336
H	-2.207531	-4.079423	-0.011852
H	-2.057346	-5.822188	-0.012692
H	-0.376694	-2.781626	-0.001896
H	2.633782	-7.640372	0.001343
H	4.905872	-6.451544	0.010315
N	-4.912971	1.627841	0.010558
O	-2.133152	-2.030932	-0.011751
N	-3.581856	-0.260777	-0.000237
C	-4.846956	0.289502	0.005298
N	-5.956243	-0.430501	0.005413
C	-5.712181	-1.754110	-0.000359
C	-4.488933	-2.410639	-0.006161
C	-3.298652	-1.624165	-0.006440
N	-6.639618	-2.759847	-0.001818
C	-5.942901	-3.952564	-0.008273
N	-4.650372	-3.781108	-0.011092
H	-4.080070	2.207702	0.011268
H	-5.822794	2.057369	0.014356
H	-2.782160	0.376983	0.000057
H	-7.640680	-2.633846	0.001300
H	-6.451731	-4.905865	-0.010609
N	1.627642	4.912345	-0.008668
O	-2.031252	2.132724	0.009102
N	-0.261089	3.581383	0.000036
C	0.289305	4.846456	-0.004349

N	-0.430669	5.955763	-0.004733
C	-1.754293	5.711755	-0.000289
C	-2.410900	4.488539	0.004475
C	-1.624485	3.298226	0.004873
N	-2.759987	6.639238	0.000679
C	-3.952747	5.942585	0.005940
N	-3.781362	4.650046	0.008332
H	2.207351	4.079319	-0.006245
H	2.057265	5.822129	-0.010525
H	0.376522	2.781609	0.000302
H	-2.633939	7.640296	-0.001894
H	-4.906023	6.451463	0.007713

Table S2. The Cartesian coordinates of the optimized geometry in Å of the G₄-Li⁺ system at M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure equals to -2177.126452 *a.u.*

N	-2.784038	4.104455	-0.888940
C	-3.187755	2.913366	-0.317610
C	-4.493529	3.008796	0.155723
N	-4.879867	4.284367	-0.145896
C	-3.817064	4.894499	-0.768802
C	-2.503483	1.683057	-0.132810
N	-3.287591	0.734829	0.502013
C	-4.581394	0.935383	0.933994
N	-5.229615	2.073782	0.774575
N	-5.164538	-0.093495	1.569986
O	-1.327608	1.415487	-0.458098
N	0.734965	3.287078	-0.501626
C	0.935571	4.580645	-0.934271
N	2.074025	5.228877	-0.775253
C	3.009030	4.493042	-0.156085
C	2.913561	3.187497	0.317861
C	1.683190	2.503214	0.133502
N	4.104625	2.784019	0.889408
C	4.894702	3.816967	0.768797
N	4.284611	4.879488	0.145368
N	-0.093308	5.163533	-1.570498
O	1.415570	1.327513	0.459367
N	3.287582	-0.734871	0.502113
C	4.581360	-0.935445	0.934155
N	5.229580	-2.073846	0.774745
C	4.493519	-3.008837	0.155828
C	3.187772	-2.913383	-0.317579
C	2.503497	-1.683076	-0.132775
N	2.784078	-4.104454	-0.888962
C	3.817088	-4.894511	-0.768781
N	4.879869	-4.284398	-0.145816
N	5.164484	0.093421	1.570186
O	1.327637	-1.415488	-0.458104
N	-0.734949	-3.287027	-0.501763
C	-0.935552	-4.580553	-0.934532
N	-2.074018	-5.228787	-0.775610
C	-3.009036	-4.492999	-0.156405
C	-2.913571	-3.187496	0.317660
C	-1.683186	-2.503211	0.133398

N	-4.104645	-2.784066	0.889221
C	-4.894727	-3.816997	0.768492
N	-4.284627	-4.879464	0.144980
N	0.093345	-5.163392	-1.570775
O	-1.415562	-1.327539	0.459373
H	1.041251	-4.790618	-1.478385
H	-0.037934	-6.131543	-1.820861
H	0.165078	-2.813838	-0.665450
H	-4.689313	-5.781993	-0.061800
H	-5.919111	-3.868552	1.109153
H	4.791529	1.041295	1.478217
H	6.132767	-0.037827	1.819776
H	2.814438	0.165075	0.666282
H	5.782503	-4.689080	0.060512
H	3.868483	-5.918892	-1.109476
H	-1.041213	4.790733	-1.478193
H	0.037969	6.131710	-1.820485
H	-0.165058	2.813908	-0.665379
H	4.689299	5.782037	-0.061324
H	5.919080	3.868495	1.109482
H	-4.791572	-1.041367	1.478031
H	-6.132832	0.037744	1.819537
H	-2.814440	-0.165114	0.666188
H	-5.782514	4.689039	0.060400
H	-3.868448	5.918889	-1.109473
Li	0.000002	0.000010	0.000729

Table S3. The Cartesian coordinates of the optimized geometry in Å of the G₄-Na⁺ system at M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure equals to -2331.854385 *a.u.*

N	-1.837006	-4.986188	0.249363
C	-0.519372	-4.573670	0.246856
C	0.337011	-5.657522	0.416060
N	-0.489406	-6.740866	0.523486
C	-1.780055	-6.279912	0.415402
C	0.055343	-3.281567	0.123725
N	1.442262	-3.316070	0.169385
C	2.200447	-4.459084	0.330241
N	1.675912	-5.664388	0.462863
N	3.529641	-4.304405	0.363657
O	-0.542255	-2.194055	-0.005361
N	-3.316089	-1.442242	-0.169564
C	-4.459152	-2.200408	-0.330181
N	-5.664492	-1.675858	-0.462401
C	-5.657612	-0.336962	-0.415456
C	-4.573711	0.519401	-0.246474
C	-3.281574	-0.055329	-0.123770
N	-4.986229	1.837035	-0.248715
C	-6.280000	1.780103	-0.414395
N	-6.740987	0.489467	-0.522477
N	-4.304478	-3.529598	-0.363851
O	-2.194031	0.542262	0.005090
N	-1.442227	3.316060	0.169478
C	-2.200388	4.459103	0.330235
N	-1.675833	5.664418	0.462665

C	-0.336933	5.657528	0.415821
C	0.519428	4.573640	0.246744
C	-0.055310	3.281532	0.123777
N	1.837069	4.986138	0.249172
C	1.780141	6.279889	0.415012
N	0.489502	6.740878	0.523058
N	-3.529584	4.304436	0.363802
O	0.542280	2.194002	-0.005206
N	3.316038	1.442232	-0.169757
C	4.459073	2.200421	-0.330457
N	5.664400	1.675892	-0.462890
C	5.657537	0.336991	-0.416073
C	4.573665	-0.519397	-0.247029
C	3.281542	0.055312	-0.124083
N	4.986190	-1.837029	-0.249453
C	6.279941	-1.780070	-0.415288
N	6.740906	-0.489419	-0.523300
N	4.304391	3.529611	-0.363960
O	2.194024	-0.542301	0.004878
H	3.418918	4.000378	-0.150615
H	5.151070	4.069928	-0.451131
H	2.400411	1.908202	-0.097679
H	7.696834	-0.190144	-0.655814
H	6.945865	-2.629691	-0.466288
H	-4.000354	3.419021	0.150223
H	-4.069882	5.151140	0.450875
H	-1.908220	2.400448	0.097336
H	0.190252	7.696803	0.655646
H	2.629776	6.945794	0.466009
H	-3.419034	-4.000378	-0.150417
H	-5.151188	-4.069894	-0.450866
H	-2.400457	-1.908226	-0.097642
H	-7.696934	0.190212	-0.654907
H	-6.945924	2.629734	-0.465231
H	4.000392	-3.418963	0.150155
H	4.069965	-5.151066	0.450969
H	1.908232	-2.400452	0.097193
H	-0.190138	-7.696769	0.656202
H	-2.629679	-6.945822	0.466523
Na	-0.000005	-0.000023	-0.000334

Table S4. The Cartesian coordinates of the optimized geometry in Å of the G_4-K^+ system at M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure equals to -2769.46756 *a.u.*

N	-2.825543	4.599416	-0.246577
C	-1.456526	4.424361	-0.223599
C	-0.800519	5.604153	-0.559051
N	-1.802504	6.505118	-0.788756
C	-2.994237	5.848053	-0.588036
C	-0.669808	3.282607	0.082710
N	0.693641	3.542265	-0.021379
C	1.242468	4.763171	-0.360717
N	0.518077	5.832909	-0.638022
N	2.578555	4.839737	-0.405888
O	-1.069849	2.152164	0.416867

N	-3.595321	0.705128	0.207457
C	-4.860258	1.251217	0.108288
N	-5.960775	0.523712	0.034848
C	-5.717384	-0.794599	0.053581
C	-4.492431	-1.447715	0.140222
C	-3.317445	-0.658215	0.249046
N	-4.662830	-2.817449	0.130867
C	-5.953609	-2.989440	0.039209
N	-6.642213	-1.799209	-0.008395
N	-4.948624	2.587890	0.108307
O	-2.145336	-1.055151	0.384287
N	-0.693588	-3.542101	-0.021824
C	-1.242398	-4.762867	-0.361680
N	-0.518011	-5.832629	-0.638889
C	0.800579	-5.604024	-0.559325
C	1.456570	-4.424372	-0.223347
C	0.669841	-3.282602	0.082891
N	2.825577	-4.599564	-0.245796
C	2.994282	-5.848145	-0.587454
N	1.802564	-6.505042	-0.788813
N	-2.578480	-4.839213	-0.407614
O	1.069869	-2.152272	0.417450
N	3.595320	-0.705189	0.208237
C	4.860204	-1.251336	0.108729
N	5.960702	-0.523880	0.034596
C	5.717344	0.794441	0.053021
C	4.492443	1.447612	0.139979
C	3.317482	0.658170	0.249540
N	4.662878	2.817337	0.130161
C	5.953624	2.989268	0.037901
N	6.642174	1.799007	-0.009654
N	4.948546	-2.588019	0.109193
O	2.145442	1.055159	0.385201
H	4.145648	-3.220418	0.034787
H	5.877304	-2.963792	-0.004793
H	2.780208	-1.332111	0.254239
H	7.642308	1.673418	-0.078587
H	6.460655	3.942814	0.000248
H	-3.217083	-4.078073	-0.160800
H	-2.960010	-5.738436	-0.656913
H	-1.318522	-2.738544	0.129645
H	1.674029	-7.471274	-1.054615
H	3.946329	-6.344862	-0.708341
H	-4.145753	3.220305	0.033716
H	-5.877445	2.963635	-0.005248
H	-2.780202	1.332071	0.253110
H	-7.642380	-1.673668	-0.076962
H	-6.460632	-3.943010	0.002051
H	3.217160	4.078350	-0.159811
H	2.960087	5.738980	-0.655107
H	1.318582	2.738765	0.130347
H	-1.673961	7.471425	-1.054284
H	-3.946286	6.344697	-0.709210
K	-0.000178	0.000027	1.430011

Table S5. The Cartesian coordinates of the S_1 optimized geometry in Å of the G_4 system at CAM-B3LYP/6-31G level of theory. Energy of the optimized structure equals to -2167.995764 *a.u.*

N	-5.069977	-2.567159	0.037919
O	-2.702714	1.435206	-0.172475
N	-3.911749	-0.537495	-0.072217
C	-5.109148	-1.231174	-0.074170
N	-6.301032	-0.632432	-0.181800
C	-6.229744	0.709881	-0.288597
C	-5.078215	1.484108	-0.294970
C	-3.817679	0.847869	-0.180031
N	-7.265651	1.603373	-0.412089
C	-6.703222	2.875262	-0.487312
N	-5.390695	2.836298	-0.419227
H	-4.225797	-3.149285	0.118100
H	-5.965439	-3.026937	0.032046
H	-3.013974	-1.053541	0.010341
H	-8.241703	1.362803	-0.440902
H	-7.301647	3.763954	-0.588929
N	2.478368	-4.205977	0.201330
O	-1.468059	-1.789939	0.121566
N	0.460424	-3.051723	0.170050
C	1.143334	-4.258572	0.214004
N	0.522934	-5.442571	0.264608
C	-0.820319	-5.345791	0.265108
C	-1.582959	-4.186261	0.218524
C	-0.931209	-2.922703	0.166756
N	-1.728338	-6.377918	0.310023
C	-2.995106	-5.816616	0.288490
N	-2.938764	-4.502563	0.233470
H	2.968630	-3.315596	0.156737
H	2.992344	-5.068838	0.220304
H	1.017905	-2.191037	0.134043
H	-1.491631	-7.354669	0.350432
H	-3.893743	-6.407676	0.314152
N	5.001698	2.590174	-0.376496
O	2.716664	-1.431472	0.097815
N	3.893674	0.545498	-0.149004
C	5.068631	1.249339	-0.326479
N	6.263357	0.660706	-0.449035
C	6.213691	-0.685583	-0.374734
C	5.084146	-1.471052	-0.186633
C	3.818449	-0.842290	-0.066355
N	7.259487	-1.571789	-0.461641
C	6.725730	-2.850537	-0.322999
N	5.422026	-2.822391	-0.156443
H	4.161329	3.157638	-0.223932
H	5.878242	3.064296	-0.516126
H	2.990396	1.062366	-0.096150
H	8.223745	-1.321798	-0.599265
H	7.336876	-3.735870	-0.353207
N	-2.403238	4.175139	-0.177860
O	1.517602	1.807260	-0.081966
N	-0.450458	2.980068	0.215549
C	-1.097676	4.193673	0.101176

N	-0.480593	5.381262	0.276722
C	0.780686	5.326503	0.829921
C	1.582717	4.149709	0.448361
C	0.965707	2.914595	0.178417
N	1.720449	6.388997	0.685525
C	2.934481	5.847381	0.370371
N	2.884409	4.533735	0.196196
H	-2.894438	3.281765	-0.268733
H	-2.902166	5.045587	-0.257619
H	-0.986084	2.115844	0.113284
H	1.530741	7.355500	0.883878

Table S6. The Cartesian coordinates of the S_1 optimized geometry in Å of the $G_4\text{-Li}^+$ system at CAM-B3LYP/6-31G level of theory. Energy of the optimized structure equals to -2175.495151 *a.u.*

N	2.509582	-4.323793	1.087084
C	1.204625	-4.168801	0.612429
C	0.620643	-5.422070	0.423737
N	1.577078	-6.332560	0.800851
C	2.696357	-5.624612	1.190548
C	0.433584	-3.020001	0.321010
N	-0.830911	-3.316616	-0.156095
C	-1.325949	-4.595749	-0.334119
N	-0.610981	-5.686734	-0.037354
N	-2.562444	-4.721342	-0.822060
O	0.788456	-1.800974	0.442863
N	3.276655	-0.836658	0.187032
C	4.547534	-1.326665	0.375787
N	5.679331	-0.663167	0.057545
C	5.472866	0.537492	-0.519606
C	4.201346	1.182662	-0.659365
C	3.023042	0.483138	-0.281842
N	4.400642	2.468695	-1.094158
C	5.744211	2.617330	-1.230877
N	6.410869	1.491954	-0.871141
N	4.665065	-2.547905	0.896236
O	1.781623	0.853805	-0.428951
N	0.818739	3.312478	-0.153885
C	1.354662	4.578932	-0.290827
N	0.668006	5.685832	0.013134
C	-0.581453	5.450155	0.441943
C	-1.205290	4.209989	0.590526
C	-0.464458	3.047824	0.286365
N	-2.513385	4.388639	1.043722
C	-2.666731	5.689932	1.171562
N	-1.519619	6.378166	0.819439
N	2.607352	4.681345	-0.746697
O	-0.859013	1.833835	0.369966
N	-3.334082	0.821481	0.143016
C	-4.607872	1.336093	0.305031
N	-5.706426	0.631070	0.016220
C	-5.455232	-0.611441	-0.424168
C	-4.207614	-1.213384	-0.596805
C	-3.051419	-0.455504	-0.307911
N	-4.372670	-2.521512	-1.055641

C	-5.673201	-2.695353	-1.163569
N	-6.373786	-1.562124	-0.792717
N	-4.720506	2.583668	0.769988
O	-1.833878	-0.829792	-0.411949
H	-3.913337	3.195797	0.962953
H	-5.657044	2.934494	0.887899
H	-2.489325	1.388905	0.355676
H	-7.372937	-1.436890	-0.785129
H	-6.160535	-3.596927	-1.491993
H	3.207210	3.871705	-0.960589
H	2.971048	5.615097	-0.845978
H	1.370323	2.449703	-0.373815
H	-1.378892	7.375187	0.828192
H	-3.562515	6.186486	1.502006
H	3.844245	-3.170005	1.082642
H	5.606070	-2.889984	1.032457
H	2.428142	-1.373844	0.430058
H	7.408806	1.350860	-0.876154
H	6.228772	3.507925	-1.590505
H	-3.181913	-3.917630	-1.009577
H	-2.899684	-5.660883	-0.955166
H	-1.398619	-2.475667	-0.381805
H	1.462210	-7.333044	0.785865
H	3.598560	-6.104464	1.528250
Li	0.011484	0.037320	-0.030490

Table S7. The Cartesian coordinates of the S_1 optimized geometry in Å of the $G_4\text{-Na}^+$ system at CAM-B3LYP/6-31G level of theory. Energy of the optimized structure equals to -2330.408807 *a.u.*

N	1.073615	5.259809	0.039633
C	-0.164564	4.617527	0.048757
C	-1.188965	5.560862	0.114875
N	-0.560029	6.780837	0.146080
C	0.803027	6.546687	0.098451
C	-0.506708	3.249534	0.004223
N	-1.874962	3.022687	0.029521
C	-2.828627	4.024178	0.096355
N	-2.509054	5.322604	0.141572
N	-4.117163	3.667947	0.116750
O	0.297572	2.260856	-0.053742
N	3.030437	1.882759	-0.057090
C	4.041293	2.831210	-0.065711
N	5.336734	2.498829	-0.075772
C	5.561855	1.176290	-0.071443
C	4.609002	0.158404	-0.058123
C	3.242463	0.510850	-0.054454
N	5.242364	-1.084824	-0.054812
C	6.532347	-0.822909	-0.066614
N	6.777366	0.538619	-0.077452
N	3.693621	4.120786	-0.063787
O	2.244870	-0.283242	-0.051833
N	1.904790	-3.032235	0.025252
C	2.843043	-4.051563	0.060602
N	2.496824	-5.343372	0.106327
C	1.172244	-5.555490	0.109251

C	0.164216	-4.594169	0.070496
C	0.531316	-3.231125	0.028952
N	-1.085066	-5.216609	0.083521
C	-0.835223	-6.509786	0.130803
N	0.522195	-6.765035	0.148333
N	4.134680	-3.714998	0.047923
O	-0.251654	-2.229195	-0.003769
N	-2.984811	-1.882381	-0.007387
C	-3.992334	-2.818043	-0.051294
N	-5.311445	-2.525489	-0.099230
C	-5.583908	-1.208434	-0.162544
C	-4.625156	-0.157112	-0.065544
C	-3.238917	-0.475450	0.063321
N	-5.279944	1.044531	-0.025871
C	-6.605609	0.754842	-0.085598
N	-6.818774	-0.585184	-0.142032
N	-3.651741	-4.105735	-0.066809
O	-2.231616	0.338500	-0.071603
H	-2.669373	-4.467666	-0.007559
H	-4.417986	-4.762169	-0.129553
H	-1.993218	-2.167205	0.014292
H	-7.708537	-1.056308	-0.188587
H	-7.394689	1.485683	-0.097963
H	4.488316	-2.744663	0.006915
H	4.790744	-4.479007	0.075858
H	2.207632	-2.040054	-0.004029
H	0.972988	-7.665002	0.182531
H	-1.573582	-7.292369	0.153161
H	2.723218	4.473828	-0.036995
H	4.454578	4.780922	-0.073822
H	2.037056	2.184069	-0.054406
H	7.673618	0.997538	-0.087410
H	7.321716	-1.554327	-0.067456
H	-4.466441	2.699338	0.074806
H	-4.780351	4.424344	0.168963
H	-2.167040	2.018938	-0.005700
H	-1.024624	7.672815	0.194423
H	1.528757	7.341190	0.109567
Na	-0.018034	0.021102	-0.104612

Table S8. The Cartesian coordinates of the S_1 optimized geometry in Å of the $G_4\text{-K}^+$ system at CAM-B3LYP/6-31G level of theory. Energy of the optimized structure equals to -2767.870073 *a.u.*

N	-1.588748	5.105375	-0.308134
C	-0.288367	4.604291	-0.272339
C	0.624533	5.617901	-0.544919
N	-0.136026	6.742490	-0.757327
C	-1.463366	6.383357	-0.603467
C	0.191350	3.304347	-0.006567
N	1.579322	3.214450	-0.047751
C	2.421595	4.282929	-0.316822
N	1.963284	5.512549	-0.577995
N	3.739648	4.061187	-0.309498
O	-0.507719	2.280379	0.260603
N	-3.162854	1.481637	-0.127855

C	-4.192126	2.339918	0.200202
N	-5.481341	1.951991	0.347930
C	-5.677189	0.632912	0.233347
C	-4.697219	-0.338949	-0.064337
C	-3.279950	0.049363	-0.094249
N	-5.296376	-1.539931	-0.294334
C	-6.618217	-1.337631	-0.151408
N	-6.889913	-0.030494	0.132853
N	-3.924052	3.632834	0.360177
O	-2.423217	-0.647401	0.612646
N	-1.543815	-3.186251	-0.009813
C	-2.378577	-4.212218	-0.422165
N	-1.932526	-5.444783	-0.686500
C	-0.607016	-5.591942	-0.532333
C	0.305571	-4.614841	-0.143873
C	-0.166195	-3.317109	0.150342
N	1.591759	-5.151460	-0.103842
C	1.457176	-6.412558	-0.456558
N	0.136732	-6.729498	-0.726406
N	-3.685619	-3.958180	-0.563982
O	0.529540	-2.325067	0.535681
N	3.225317	-1.544748	0.275040
C	4.302561	-2.408205	0.135846
N	5.559968	-1.973079	0.003826
C	5.679660	-0.635788	-0.007029
C	4.655423	0.300612	0.109694
C	3.331511	-0.155248	0.288930
N	5.178405	1.592115	0.045109
C	6.477207	1.436760	-0.103939
N	6.831775	0.098960	-0.138543
N	4.063438	-3.723342	0.137208
O	2.296468	0.559206	0.469481
H	3.131300	-4.165826	0.139907
H	4.874937	-4.313502	0.045202
H	2.269810	-1.934943	0.365285
H	7.756952	-0.284539	-0.242812
H	7.198678	2.230148	-0.193393
H	-4.147661	-3.052018	-0.436308
H	-4.248070	-4.735682	-0.870756
H	-1.949369	-2.246023	0.197819
H	-0.230046	-7.621969	-1.014027
H	2.253959	-7.131429	-0.535980
H	-3.018734	4.097242	0.133083
H	-4.705014	4.213454	0.632554
H	-2.206056	1.861099	-0.143782
H	-7.796282	0.386639	0.275650
H	-7.373554	-2.099325	-0.231867
H	4.189872	3.150958	-0.127635
H	4.320748	4.859135	-0.510895
H	1.975964	2.271825	0.122709
H	0.225549	7.655342	-0.981200
H	-2.271291	7.085153	-0.715947
K	-0.077952	0.025640	1.480201