Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 85 (8) S376–S388 (2020) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Properties of the excited electronic states of guanine quartet complexes with alkali metal cations

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J. Serb. Chem. Soc. 85 (8) (2020) 1021–1032

TABLE S-I. The Cartesian coordinates of the optimized geometry in Å of the G_4 system at the M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure is equal 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	5.94315	3.952567	–0.009712
N	4.65061	3.781201	–0.00733
H	4.079938	–2.207575	0.009577
H	5.822704	–2.057433	0.007095
H	2.782192	–0.376716	0.006288
H	7.64087	2.633743	–0.008343
H	6.45204	4.905834	–0.0132
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	2.41076	–4.488612	0.005165
C	1.624366	–3.298284	0.0043
N	2.759836	–6.639313	0.003108

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C	3.9526	–5.94266	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	–1.75411	–0.000359
C	–4.488933	–2.410639	–0.006161
C	–3.298652	–1.624165	–0.00644
N	–6.639618	–2.759847	–0.001818
C	–5.942901	–3.952564	–0.008273
N	–4.650372	–3.781108	–0.011092
H	–4.08007	2.207702	0.011268
H	–5.822794	2.057369	0.014356
H	–2.78216	0.376983	0.000057
H	–7.64068	–2.633846	0.0013
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	–2.4109	4.488539	0.004475
C	–1.624485	3.298226	0.004873
N	–2.759987	6.639238	0.000679
C	–3.952747	5.942585	0.00594
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 S-II. The Cartesian coordinates of the optimized geometry in Å of the G_4–Li^+ system at the M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure is equal to –2177.126452 a.u.

N	–2.784038	4.104455	–0.88894
C	–3.187755	2.913366	–0.31761
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	–0.13281
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	3.00903	4.493042	–0.156085
C	2.913561	3.187497	0.317861
C	1.68319	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	1.41557	1.327513	0.459367
N	3.287582	–0.734871	0.502113
C	4.58136	–0.935445	0.934155
N	5.22958	–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	–0.77561
C	–3.009036	–4.492999	–0.156405
C	–2.913571	–3.187496	0.31766
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	0.14498

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	–0.66545
H	–4.689313	–5.781993	–0.0618
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	–4.68908	0.060512
H	3.868483	–5.918892	–1.109476
H	–1.041213	4.790733	–1.478193
H	0.037969	6.13171	–1.820485
H	–0.165058	2.813908	–0.665379
H	4.689299	5.782037	–0.061324
H	5.91908	3.868495	1.109482
H	–4.791572	–1.041367	1.478031
H	–6.132832	0.037744	1.819537
H	–2.81444	–0.165114	0.666188
H	–5.782514	4.689039	0.0604
H	–3.868448	5.918889	–1.109473
Li	0.000002	0.00001	0.000729

TABLE S-III. The Cartesian coordinates of the optimized geometry in Å of the G_4–Na^+ system at the M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure is equal to –2331.854385 a.u.

N	–1.837006	–4.986188	0.249363
C	–0.519372	–4.57367	0.246856
C	0.337011	–5.657522	0.41606
N	–0.489406	–6.740866	0.523486
C	–1.780055	–6.279912	0.415402
C	0.055343	–3.281567	0.123725
N	1.442262	–3.31607	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	–0.12377
N	–4.986229	1.837035	–0.248715
C	–6.28	1.780103	–0.414395

N	–6.740987	0.489467	–0.522477
N	–4.304478	–3.529598	–0.363851
O	–2.194031	0.542262	0.00509
N	–1.442227	3.31606	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	4.57364	0.246744
C	–0.05531	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	0.54228	2.194002	–0.005206
N	3.316038	1.442232	–0.169757
C	4.459073	2.200421	–0.330457
N	5.6644	1.675892	–0.46289
C	5.657537	0.336991	–0.416073
C	4.573665	–0.519397	–0.247029
C	3.281542	0.055312	–0.124083
N	4.98619	–1.837029	–0.249453
C	6.279941	–1.78007	–0.415288
N	6.740906	–0.489419	–0.5233
N	4.304391	3.529611	–0.36396
O	2.194024	–0.542301	0.004878
H	3.418918	4.000378	–0.150615
H	5.15107	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	5.15114	0.450875
H	–1.90822	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 S-IV. The Cartesian coordinates of the optimized geometry in Å of the G_4–K^+ system at the M06-2X/6-311+G(d,p) level of theory. Energy of the optimized structure is equal 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	0.08271
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	–4.66283	–2.817449	0.130867
C	–5.953609	–2.98944	0.039209
N	–6.642213	–1.799209	–0.008395
N	–4.948624	2.58789	0.108307
O	–2.145336	–1.055151	0.384287
N	–0.693588	–3.542101	–0.021824
C	–1.242398	–4.762867	–0.36168
N	–0.518011	–5.832629	–0.638889
C	0.800579	–5.604024	–0.559325
C	1.45657	–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	–2.57848	–4.839213	–0.407614
O	1.069869	–2.152272	0.41745
N	3.59532	–0.705189	0.208237
C	4.860204	–1.251336	0.108729
N	5.960702	–0.52388	0.034596
C	5.717344	0.794441	0.053021
C	4.492443	1.447612	0.139979
C	3.317482	0.65817	0.24954
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	–0.1608
H	–2.96001	–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	0.25311
H	–7.64238	–1.673668	–0.076962
H	–6.460632	–3.94301	0.002051
H	3.21716	4.07835	–0.159811
H	2.960087	5.73898	–0.655107
H	1.318582	2.738765	0.130347
H	–1.673961	7.471425	–1.054284
H	–3.946286	6.344697	–0.70921
K	–0.000178	0.000027	1.430011

TABLE S-V. The Cartesian coordinates of the S1 optimized geometry in Å of the G_4 system at the CAMB3LYP/6-31G level of theory. Energy of the optimized structure is 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	–0.07417
N	–6.301032	–0.632432	–0.1818
C	–6.229744	0.709881	–0.288597
C	–5.078215	1.484108	–0.29497
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	0.1181
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	0.20133
O	–1.468059	–1.789939	0.121566
N	0.460424	–3.051723	0.17005
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	0.28849
N	–2.938764	–4.502563	0.23347
H	2.96863	–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	–0.84229	–0.066355
N	7.259487	–1.571789	–0.461641
C	6.72573	–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	–0.09615
H	8.223745	–1.321798	–0.599265
H	7.336876	–3.73587	–0.353207
N	–2.403238	4.175139	–0.17786
O	1.517602	1.80726	–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	7.3555	0.883878
H	3.830392	6.437971	0.269863

TABLE S-VI. The Cartesian coordinates of the S1 optimized geometry in Å of the G_4–Li^+ system at the CAMB3LYP/6-31G level of theory. Energy of the optimized structure is equal to –2175.495151 a.u.

N	2.509582	–4.323793	1.087084
C	1.204625	–4.168801	0.612429
C	0.620643	–5.42207	0.423737
N	1.577078	–6.33256	0.800851
C	2.696357	–5.624612	1.190548
C	0.433584	–3.020001	0.32101
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	–0.82206
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	2.61733	–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	–1.20529	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	0.63107	0.01622
C	–5.455232	–0.611441	–0.424168
C	–4.207614	–1.213384	–0.596805
C	–3.051419	–0.455504	–0.307911
N	–4.37267	–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	–1.43689	–0.785129
H	–6.160535	–3.596927	–1.491993
H	3.20721	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	5.60607	–2.889984	1.032457
H	2.428142	–1.373844	0.430058
H	7.408806	1.35086	–0.876154
H	6.228772	3.507925	–1.590505
H	–3.181913	–3.91763	–1.009577
H	–2.899684	–5.660883	–0.955166
H	–1.398619	–2.475667	–0.381805
H	1.46221	–7.333044	0.785865
H	3.59856	–6.104464	1.52825
Li	0.011484	0.03732	–0.03049

TABLE S-VII. The Cartesian coordinates of the S1 optimized geometry in Å of the G_4-Na^+ system at the CAMB3LYP/6-31G level of theory. Energy of the optimized structure is equal to –2330.408807 a.u.

N	1.073589	5.259814	0.039633
C	–0.164587	4.617526	0.048757
C	–1.188992	5.560856	0.114875
N	–0.560062	6.780834	0.14608
C	0.802995	6.546691	0.098451
C	–0.506724	3.249532	0.004223
N	–1.874977	3.022678	0.029521
C	–2.828647	4.024164	0.096355
N	–2.50908	5.322592	0.141572
N	–4.117181	3.667927	0.11675
O	0.297561	2.260858	–0.053742
N	3.030428	1.882774	–0.05709
C	4.041279	2.83123	–0.065711
N	5.336722	2.498855	–0.075772
C	5.561849	1.176318	–0.071443
C	4.609001	0.158427	–0.058123
C	3.24246	0.510866	–0.054454
N	5.242369	–1.084798	–0.054812
C	6.532351	–0.822877	–0.066614
N	6.777363	0.538653	–0.077452

N	3.693601	4.120804	–0.063787
O	2.244871	–0.283231	–0.051833
N	1.904805	–3.032226	0.025252
C	2.843063	–4.051549	0.060602
N	2.49685	–5.34336	0.106327
C	1.172271	–5.555484	0.109251
C	0.164239	–4.594168	0.070496
C	0.531332	–3.231122	0.028952
N	–1.08504	–5.216614	0.083521
C	–0.835191	–6.50979	0.130803
N	0.522228	–6.765032	0.148333
N	4.134698	–3.714978	0.047923
O	–0.251643	–2.229196	–0.003769
N	–2.984802	–1.882396	–0.007387
C	–3.99232	–2.818063	–0.051294
N	–5.311432	–2.525515	–0.09923
C	–5.583902	–1.208462	–0.162544
C	–4.625155	–0.157135	–0.065544
C	–3.238915	–0.475466	0.063321
N	–5.279949	1.044505	–0.025871
C	–6.605613	0.754809	–0.085598
N	–6.818771	–0.585218	–0.142032
N	–3.651721	–4.105753	–0.066809
O	–2.231618	0.338489	–0.071603
H	–2.669351	–4.467679	–0.007559
H	–4.417962	–4.762191	–0.129553
H	–1.993207	–2.167215	0.014292
H	–7.708532	–1.056346	–0.188587
H	–7.394696	1.485646	–0.097963
H	4.48833	–2.744641	0.006915
H	4.790766	–4.478983	0.075858
H	2.207642	–2.040043	–0.004029
H	0.973026	–7.664997	0.182531
H	–1.573546	–7.292377	0.153161
H	2.723196	4.473842	–0.036995
H	4.454554	4.780944	–0.073822
H	2.037045	2.184079	–0.054406
H	7.673613	0.997576	–0.08741
H	7.321724	–1.554291	–0.067456
H	–4.466454	2.699316	0.074806
H	–4.780373	4.42432	0.168963
H	–2.16705	2.018927	–0.0057
H	–1.024662	7.67281	0.194423
H	1.528721	7.341198	0.109567
Na	–0.018034	0.021102	–0.104612

TABLE S-VIII. The Cartesian coordinates of the S1 optimized geometry in Å of the G_4–K^+ system at the CAMB3LYP/6-31G level of theory. Energy of the optimized structure is equal 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	6.74249	–0.757327
C	–1.463366	6.383357	–0.603467
C	0.19135	3.304347	–0.006567
N	1.579322	3.21445	–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	0.34793
C	–5.677189	0.632912	0.233347
C	–4.697219	–0.338949	–0.064337
C	–3.27995	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	–0.6865
C	–0.607016	–5.591942	–0.532333
C	0.305571	–4.614841	–0.143873
C	–0.166195	–3.317109	0.150342
N	1.591759	–5.15146	–0.103842
C	1.457176	–6.412558	–0.456558
N	0.136732	–6.729498	–0.726406
N	–3.685619	–3.95818	–0.563982
O	0.52954	–2.325067	0.535681
N	3.225317	–1.544748	0.27504
C	4.302561	–2.408205	0.135846
N	5.559968	–1.973079	0.003826
C	5.67966	–0.635788	–0.007029
C	4.655423	0.300612	0.109694
C	3.331511	–0.155248	0.28893
N	5.178405	1.592115	0.045109
C	6.477207	1.43676	–0.103939
N	6.831775	0.09896	–0.138543
N	4.063438	–3.723342	0.137208

O	2.296468	0.559206	0.469481
H	3.1313	–4.165826	0.139907
H	4.874937	–4.313502	0.045202
H	2.26981	–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	–4.24807	–4.735682	–0.870756
H	–1.949369	–2.246023	0.197819
H	–0.230046	–7.621969	–1.014027
H	2.253959	–7.131429	–0.53598
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	0.27565
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	–0.9812
H	–2.271291	7.085153	–0.715947
K	–0.077952	0.02564	1.480201