

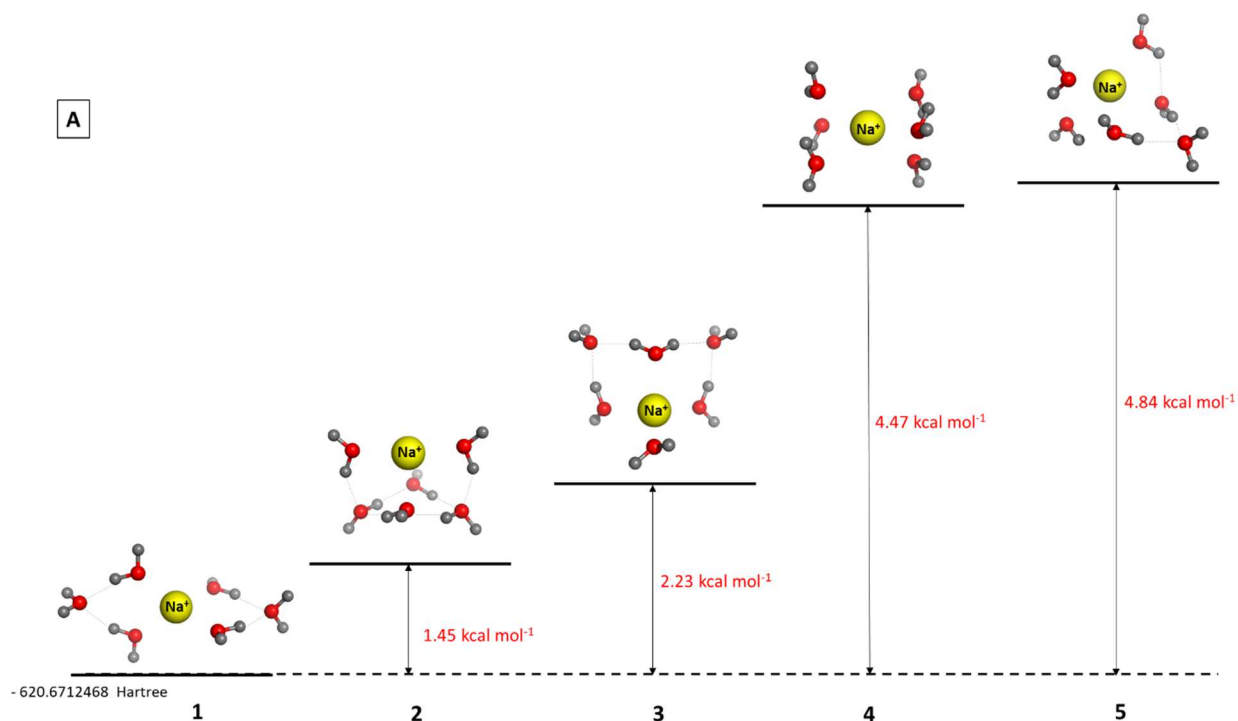
Theoretical assessment of the ligand/metal/quadruplex recognition in the non-canonical nucleic acids structures

Nikoleta Kircheva ¹, Stefan Dobrev ¹, Vladislava Petkova ¹, Snezhana Bakalova ², Jose Kaneti ², Silvia Angelova ^{1,*}

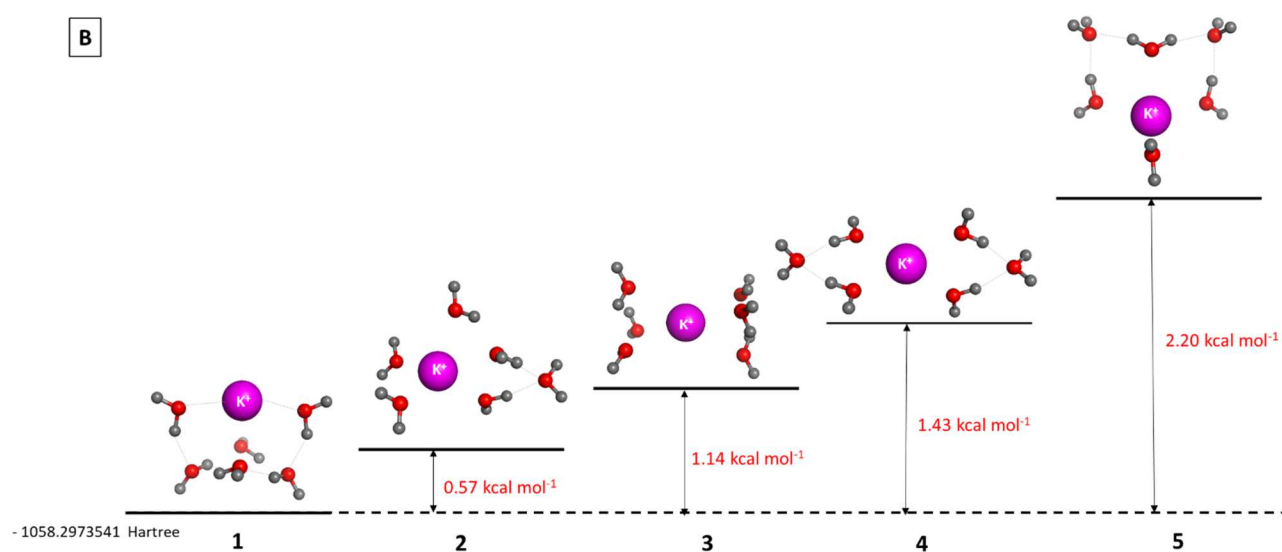
¹ Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria; nkircheva@iomt.bas.bg (N. K.), sdobrev@iomt.bas.bg (S. D.), vpetkova@iomt.bas.bg (V. P.)

² Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria; Snezhana.Bakalova@orgchm.bas.bg (S. B.), Jose.Kaneti@orgchm.bas.bg (J. K.)

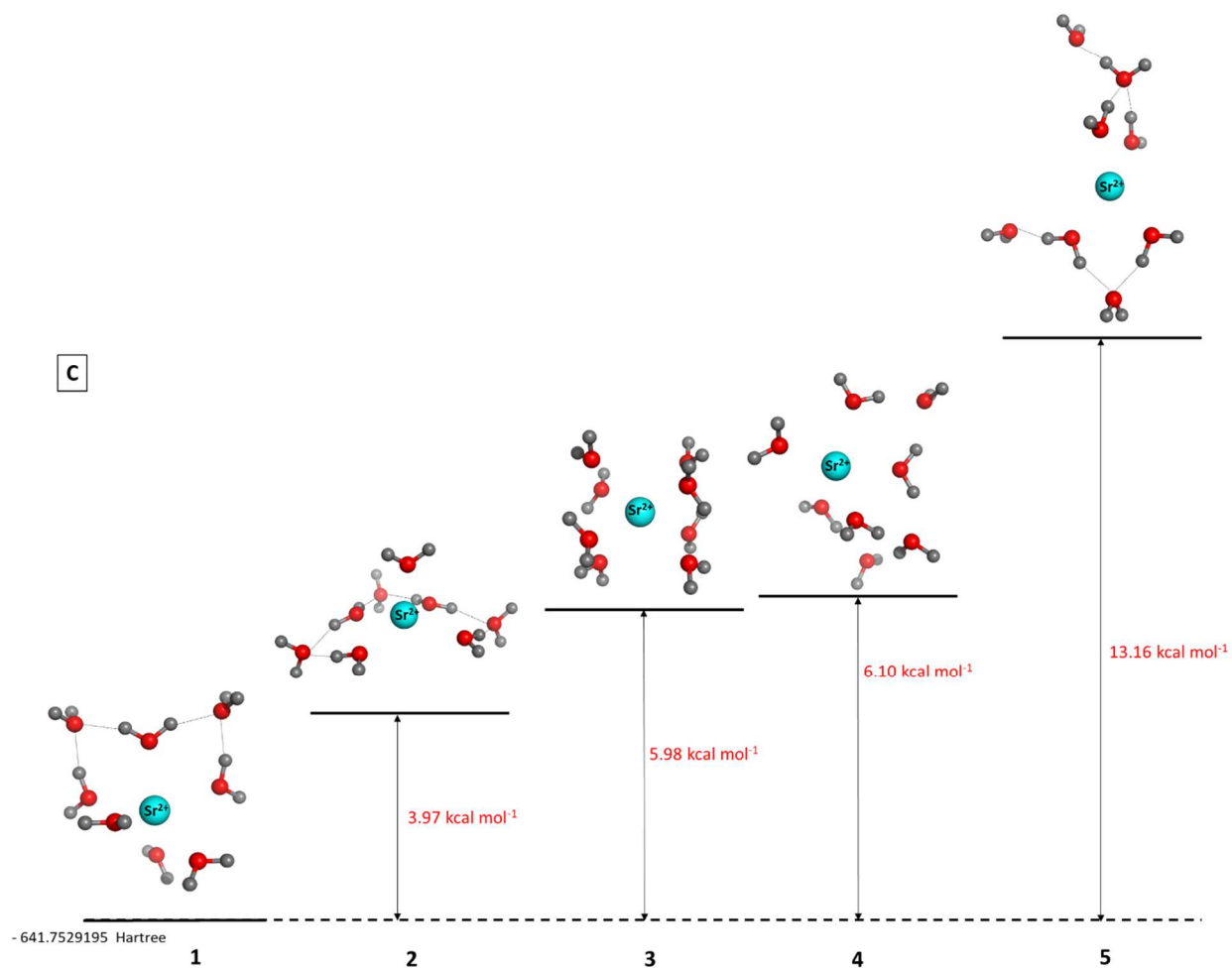
Correspondence: sea@iomt.bas.bg



B



C



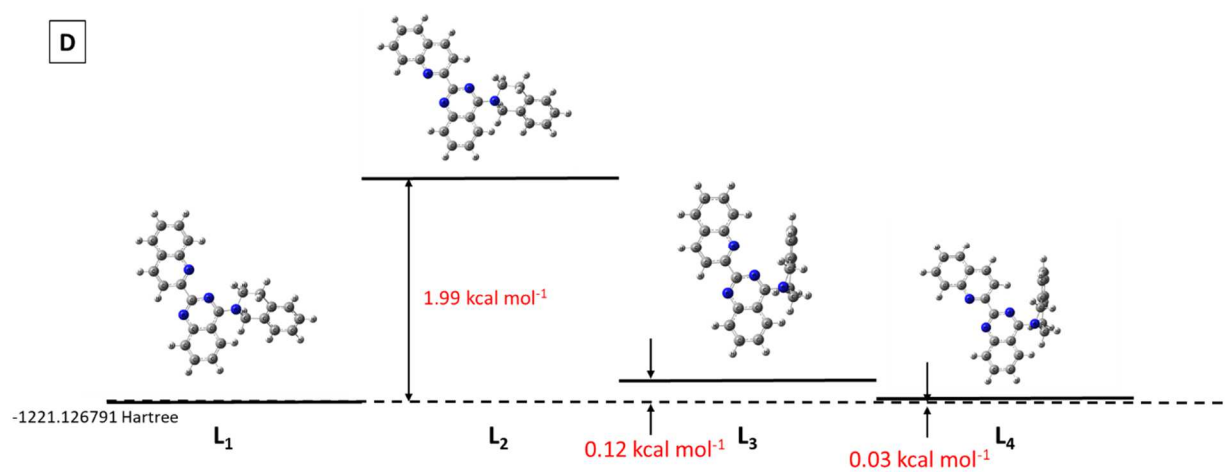


Figure S1. Structures and relative stabilities of the hydrated Na^+ , K^+ and Sr^{2+} ion clusters: $\text{Na}(\text{H}_2\text{O})_6^{1+}$ (A), $\text{K}(\text{H}_2\text{O})_6^{1+}$ (B) and $\text{Sr}(\text{H}_2\text{O})_8^{2+}$ (C); Structures and relative stabilities of rotamers of Ligand L. All structures are optimized at wb97xd/6-31g(d,p) level of theory.

Table S1. ΔH , $T\Delta S$, ΔG^1 , ΔG^2 , ΔG^4 , and ΔG^{30} values in kcal mol⁻¹ calculated at the **wB97XD/6-31G(d,p)//wB97XD/6-31G(d,p)** and **wB97XD/6-31+G(d,p)//wB97XD/6-31G(d,p)** levels of theory for reaction **R1**: substitution of K⁺ by Na⁺; reaction **R2**: substitution of K⁺ by Sr²⁺; reaction **R3**: addition of the ligand 4-(3,4-dihydroisoquinolin-2-yl)-2-(quinolin-2-yl)quinazoline L to the K@GQ¹⁺ constructs.

		wB97XD/6-31G(d,p)//wB97XD/6-31G(d,p)						wB97XD/6-31+G(d,p)//wB97XD/6-31G(d,p)					
		ΔH	$T\Delta S$	ΔG^1	ΔG^2	ΔG^4	ΔG^{30}	ΔH	$T\Delta S$	ΔG^1	ΔG^2	ΔG^4	ΔG^{30}
GG	R1	-4.4	-7.0	2.6	3.0	3.8	4.2	-3.1	-7.0	3.9	5.3	5.9	6.4
	R2	-11.3	9.7	-21.0	-7.5	2.8	13.2	-21.8	9.7	-31.5	-13.9	-3.2	7.5
	R3	-39.4	-19.2	-20.2	-2.4	-1.2	-0.8	-36.8	-19.2	-17.6	-0.1	2.1	3.4
AG	R1	-9.2	-7.5	-1.7	-1.9	-0.7	0.4	-8.7	-7.5	-1.3	-1.1	-0.4	0.6
	R2	13.4	11.6	1.8	1.3	11.7	20.2	2.8	11.6	-8.9	-0.9	6.6	13.0
	R3	-40.4	-18.3	-22.1	-4.9	-2.8	-1.3	-37.3	-18.3	-19.0	-2.8	0.2	2.6
CG	R1	-5.8	-8.3	2.5	1.3	2.3	3.1	-4.2	-8.3	4.1	3.1	3.6	4.7
	R2	-4.4	12.5	-16.9	-9.5	-0.3	8.5	-15.4	12.5	-27.9	-15.5	-6.7	2.4
	R3	-31.9	-17.7	-14.2	-0.7	1.6	0.7	-30.2	-17.7	-12.5	1.4	4.0	4.1
TG	R1	-2.8	-6.1	3.3	3.5	4.4	4.9	-1.6	-6.1	4.5	5.7	6.2	6.8
	R2	-5.3	9.6	-14.9	-6.5	2.0	12.1	-15.9	9.6	-25.5	-10.6	-2.2	6.4
	R3	-35.7	-19.2	-16.5	-2.4	-1.3	-1.3	-32.3	-19.2	-13.1	1.6	3.5	4.1
UG	R1	-2.3	-7.6	5.3	5.2	6.1	6.8	-0.6	-7.6	7.0	7.7	8.2	8.9
	R2	-5.8	8.0	-13.8	-3.5	5.6	15.3	-17.3	8.0	-25.3	-10.5	-1.2	8.9
	R3	-37.7	-21.6	-16.1	-3.0	-1.1	0.3	-34.4	-21.6	-12.8	0.8	3.6	5.8

Methodology adopted for implicit solvent calculations

For the implicit solvation calculations, the "generic" solvent option was used with Eps (2/4/30) and EpsInf (2) values specified. As we are aware that 7 parameters are needed to define a solvent for SMD, additional calculations were performed with the following pre-defined solvents (n-dodecane, $\epsilon=2.0060$; diethylether, $\epsilon=4.2400$; propanonitrile: $\epsilon=29.324$) for reaction (1). These particular solvents were chosen as they are widely accepted and applied in other articles when simulating biological environment [39,42]. The results show that for each couple (incomplete specification of generic solvent/pre-defined solvent with close ϵ value) there is a difference of about 0.5 kcal mol⁻¹ for the wB97XD/6-31G(d,p)//wB97XD/6-31G(d,p) calculations: $\Delta G^2=0.3$ vs 0.1/ $\Delta G^4=0.6$ vs 1.1/ $\Delta G^{30}=1.0$ vs 1.5, respectively, and about 0.1-0.2 kcal mol⁻¹ for the wB97XD/6-311G(d,p)//wB97XD/6-31G(d,p) calculations: $\Delta G^2=0.9$ vs 1.0/ $\Delta G^4=1.3$ vs 1.5/ $\Delta G^{30}=1.7$ vs 1.9 kcal mol⁻¹, respectively. Note that these differences do not change the observed trends, but rather bring stronger evidence to the drawn conclusions. As we have further performed higher-level calculations, we believe that the definition of the solvent does not play a significant role in the obtained results, as seen in our previous work where the same scheme was applied [63].

Starting geometries for K@GG¹⁺, K@AG¹⁺, K@CG¹⁺, K@TG¹⁺ and K@UG¹⁺ optimization

K@GG¹⁺:

7	-6.998881000	-0.528519000	-1.146479000
6	-6.706627000	0.764359000	-1.343028000
6	-5.487695000	1.334703000	-1.673569000
6	-4.353361000	0.487503000	-1.800931000
7	-4.681373000	-0.850984000	-1.592501000
6	-5.941179000	-1.313536000	-1.293625000
7	-7.571843000	1.822026000	-1.254280000
6	-6.851961000	2.958665000	-1.536506000
7	-5.599285000	2.705124000	-1.792795000
7	-6.087061000	-2.635588000	-1.136603000
7	-1.746917290	3.138109430	-2.781711460
6	-0.406634290	2.790648430	-2.940509460
6	0.394679710	3.917967430	-3.270385460
6	-0.217987290	5.156081430	-3.381864460
7	-1.514944290	5.463217430	-3.241371460
6	-2.253389290	4.406757430	-2.934457460
7	1.754565710	4.017899430	-3.481768460
6	1.961789710	5.284360430	-3.710403460
7	0.803622710	6.024509430	-3.660937460
8	-0.036242290	1.621145430	-2.789458460
7	-3.573188290	4.562983430	-2.765036460
7	2.297365710	0.078986430	-3.243503460
6	3.557549710	0.532026430	-3.554466460
7	4.621855710	-0.249714570	-3.633755460
6	4.338291710	-1.529662570	-3.353798460
6	3.108489710	-2.097320570	-3.059965460
6	1.969993710	-1.251077570	-2.987489460
7	3.234011710	-3.451204570	-2.820132460
6	4.508236710	-3.692733570	-2.959613460
7	5.223656710	-2.570723570	-3.294942460
7	3.691567710	1.844865430	-3.795403460
8	0.803899710	-1.569211570	-2.722222460
7	-0.718155290	-3.913770570	-2.361722460
6	-2.022466290	-3.558617570	-2.034129460
6	-2.842777290	-4.699804570	-1.821026460
6	-2.267838290	-5.956546570	-1.928850460
7	-1.003849290	-6.274090570	-2.233840460

6	-0.249566290	-5.203271570	-2.440040460
7	-4.172354290	-4.794126570	-1.462649460
6	-4.397375290	-6.074112570	-1.356074460
7	-3.280489290	-6.828370570	-1.626056460
8	-2.352713290	-2.368476570	-1.950174460
7	1.040621710	-5.367921570	-2.761836460
1	-0.069379290	-3.124832570	-2.516593460
1	1.739252710	-4.615777570	-2.748306460
1	1.364772710	-6.319818570	-2.743201460
1	1.515600710	0.746225430	-3.163545460
1	4.632011710	2.159533430	-3.958899460
1	2.953149710	2.538934430	-3.644920460
1	0.702983710	7.010037430	-3.841967460
1	-2.379980290	2.360671430	-2.536709460
1	-3.914215290	5.502957430	-2.866726460
1	-4.208905290	3.835885430	-2.419380460
1	-3.901561000	-1.520793000	-1.705539000
1	-7.026326000	-2.950500000	-0.966782000
1	-5.341260000	-3.329819000	-1.265824000
1	-7.306822000	3.937801000	-1.530852000
1	-5.340106290	-6.526186570	-1.086069460
1	4.982258710	-4.653590570	-2.827294460
1	2.920292710	5.737308430	-3.915503460
1	-8.558281000	1.758595000	-1.062052000
1	-3.213347290	-7.833052570	-1.643899460
1	6.219962710	-2.500603570	-3.420375460
19	-0.886387290	-0.250248570	-0.980395460
7	-4.335056290	-4.433838570	1.878950540
6	-5.032706290	-3.293713570	1.960617540
6	-4.597541290	-1.994997570	1.745592540
6	-3.250291290	-1.789110570	1.342227540
7	-2.552394290	-2.990571570	1.237908540
6	-3.078764290	-4.231687570	1.509967540
7	-6.358687290	-3.169398570	2.276388540
6	-6.660337290	-1.829563570	2.235012540
7	-5.629009290	-1.095640570	1.923547540
8	-2.690483290	-0.712854570	1.093786540
7	-2.254114290	-5.282055570	1.411457540
7	-3.432058290	2.022927430	1.013563540
6	-2.313057290	2.712864430	0.562214540
6	-2.573018290	4.100946430	0.408431540
6	-3.838693290	4.575039430	0.710231540
7	-4.900882290	3.893451430	1.155489540
6	-4.646839290	2.599832430	1.296444540
7	-1.735932290	5.129167430	0.030026540
6	-2.478968290	6.199686430	0.086545540
7	-3.764169290	5.925057430	0.491056540
8	-1.249658290	2.119366430	0.344462540
7	-5.618667290	1.791719430	1.736081540
7	1.452563710	2.733455430	-0.139139460
6	2.001535710	3.984645430	-0.293345460
7	3.286150710	4.204480430	-0.517352460
6	3.992837710	3.065919430	-0.595636460
6	3.547066710	1.764619430	-0.436762460
6	2.167506710	1.537719430	-0.193016460

7	4.573948710	0.865815430	-0.613816460
6	5.618020710	1.598496430	-0.876858460
7	5.325274710	2.942898430	-0.881936460
7	1.170838710	5.035398430	-0.185324460
8	1.592097710	0.451909430	-0.049192460
7	2.278826710	-2.308266570	0.112908540
6	1.113404710	-3.048422570	0.252867540
6	1.383064710	-4.424806570	0.470335540
6	2.703813710	-4.826594570	0.585786540
7	3.813793710	-4.089267570	0.482633540
6	3.554821710	-2.814987570	0.224144540
7	0.523766710	-5.481985570	0.683869540
6	1.303483710	-6.504884570	0.903369540
7	2.634826710	-6.168660570	0.856053540
8	0.003190710	-2.500778570	0.203829540
7	4.571721710	-1.963326570	0.030590540
1	2.149646710	-1.289415570	0.025389540
1	4.413955710	-0.967419570	-0.143394460
1	5.408373710	-2.160413570	0.561515540
1	0.437711710	2.632376430	0.017187540
1	1.587004710	5.929785430	-0.379788460
1	0.148531710	4.962957430	-0.164340460
1	-4.509911290	6.585773430	0.637204540
1	-3.295374290	1.008945430	1.145089540
1	-6.505830290	2.231901430	1.906427540
1	-5.541513290	0.769388430	1.790249540
1	-1.576458290	-2.913136570	0.901487540
1	-2.681156290	-6.179917570	1.561266540
1	-1.286227290	-5.245626570	1.067499540
1	-7.654148290	-1.461110570	2.441248540
1	0.975332710	-7.514859570	1.100016540
1	6.614375710	1.227513430	-1.065243460
1	-2.158699290	7.200468430	-0.161777460
1	-6.977677290	-3.926304570	2.517248540
1	3.423141710	-6.775026570	1.014876540
1	5.973124710	3.702407430	-1.010903460
8	-3.188013290	0.819136430	-2.054956460

K@AG¹⁺:

7	3.822000000	6.806000000	-4.639000000
6	4.073000000	6.527000000	-3.352000000
7	3.002000000	6.347000000	-2.624000000
6	1.965000000	6.465000000	-3.565000000
6	0.555000000	6.350000000	-3.547000000
7	-0.157000000	5.979000000	-2.505000000
7	-0.167000000	6.511000000	-4.663000000
6	0.472000000	6.761000000	-5.798000000
7	1.781000000	6.877000000	-5.975000000
6	2.471000000	6.723000000	-4.810000000
1	5.125000000	6.488000000	-3.123000000
1	-1.140000000	5.867000000	-2.753000000
1	0.307000000	5.415000000	-1.804000000
1	-0.114000000	6.899000000	-6.694000000
7	6.074000000	3.476000000	-2.459000000
6	5.289000000	3.372000000	-3.577000000

7	4.004000000	3.394000000	-3.345000000
6	3.935000000	3.505000000	-1.951000000
6	2.824000000	3.672000000	-1.057000000
8	1.642000000	3.858000000	-1.333000000
7	3.173000000	3.649000000	0.278000000
6	4.453000000	3.644000000	0.714000000
7	4.641000000	3.652000000	2.006000000
7	5.519000000	3.608000000	-0.081000000
6	5.198000000	3.529000000	-1.405000000
1	5.711000000	3.331000000	-4.570000000
1	2.408000000	3.677000000	0.931000000
1	3.871000000	3.570000000	2.671000000
1	5.601000000	3.572000000	2.282000000
7	-4.797000000	6.235000000	-4.171000000
6	-3.525000000	5.846000000	-4.341000000
7	-2.831000000	5.773000000	-3.234000000
6	-3.781000000	6.118000000	-2.255000000
6	-3.791000000	6.254000000	-0.848000000
7	-2.757000000	6.050000000	-0.064000000
7	-4.917000000	6.549000000	-0.186000000
6	-6.032000000	6.716000000	-0.883000000
7	-6.176000000	6.636000000	-2.199000000
6	-5.003000000	6.341000000	-2.827000000
1	-3.283000000	5.644000000	-5.373000000
1	-3.024000000	6.040000000	0.920000000
1	-1.950000000	5.572000000	-0.429000000
1	-6.934000000	6.967000000	-0.347000000
7	-2.498000000	2.852000000	-6.524000000
6	-3.599000000	2.712000000	-5.719000000
7	-3.347000000	2.762000000	-4.439000000
6	-1.958000000	2.934000000	-4.397000000
6	-1.048000000	3.104000000	-3.303000000
8	-1.302000000	3.190000000	-2.109000000
7	0.276000000	3.206000000	-3.677000000
6	0.680000000	3.269000000	-4.966000000
7	1.959000000	3.413000000	-5.173000000
7	-0.130000000	3.172000000	-6.015000000
6	-1.437000000	2.997000000	-5.669000000
1	-4.597000000	2.613000000	-6.123000000
1	0.932000000	3.303000000	-2.920000000
1	2.631000000	3.399000000	-4.406000000
1	2.233000000	3.377000000	-6.138000000
7	-4.516000000	6.220000000	4.533000000
6	-4.655000000	5.834000000	3.257000000
7	-3.545000000	5.857000000	2.565000000
6	-2.596000000	6.260000000	3.519000000
6	-1.201000000	6.492000000	3.533000000
7	-0.408000000	6.356000000	2.493000000
7	-0.560000000	6.812000000	4.664000000
6	-1.268000000	6.911000000	5.781000000
7	-2.576000000	6.740000000	5.923000000
6	-3.182000000	6.422000000	4.744000000
1	-5.666000000	5.555000000	3.005000000
1	0.578000000	6.427000000	2.744000000
1	-0.744000000	5.887000000	1.669000000

1	-0.753000000	7.183000000	6.689000000
7	-6.498000000	2.615000000	2.140000000
6	-5.700000000	2.592000000	3.254000000
7	-4.428000000	2.766000000	3.017000000
6	-4.381000000	2.888000000	1.623000000
6	-3.291000000	3.119000000	0.721000000
8	-2.117000000	3.339000000	0.985000000
7	-3.647000000	3.112000000	-0.611000000
6	-4.925000000	2.999000000	-1.040000000
7	-5.112000000	2.984000000	-2.332000000
7	-5.976000000	2.849000000	-0.240000000
6	-5.642000000	2.790000000	1.082000000
1	-6.106000000	2.481000000	4.249000000
1	-2.887000000	3.177000000	-1.266000000
1	-4.334000000	2.956000000	-2.991000000
1	-6.058000000	2.798000000	-2.609000000
7	4.216000000	6.835000000	4.143000000
6	2.933000000	6.483000000	4.302000000
7	2.254000000	6.408000000	3.186000000
6	3.230000000	6.690000000	2.214000000
6	3.268000000	6.783000000	0.803000000
7	2.235000000	6.606000000	0.010000000
7	4.412000000	7.035000000	0.153000000
6	5.519000000	7.192000000	0.865000000
7	5.639000000	7.145000000	2.185000000
6	4.449000000	6.895000000	2.800000000
1	2.666000000	6.324000000	5.334000000
1	2.485000000	6.584000000	-0.979000000
1	1.364000000	6.268000000	0.376000000
1	6.435000000	7.412000000	0.338000000
7	2.078000000	3.265000000	6.233000000
6	3.190000000	3.286000000	5.432000000
7	2.938000000	3.371000000	4.154000000
6	1.538000000	3.390000000	4.108000000
6	0.619000000	3.503000000	3.015000000
8	0.862000000	3.702000000	1.832000000
7	-0.707000000	3.393000000	3.378000000
6	-1.125000000	3.309000000	4.661000000
7	-2.411000000	3.206000000	4.851000000
7	-0.313000000	3.279000000	5.714000000
6	1.009000000	3.312000000	5.376000000
1	4.190000000	3.275000000	5.840000000
1	-1.367000000	3.384000000	2.618000000
1	-3.059000000	3.094000000	4.071000000
1	-2.677000000	3.035000000	5.804000000
1	-5.249246750	6.337625580	5.202711450
1	-5.466619800	6.413307880	-4.891982400
1	4.497338720	7.032189290	-5.340965820
1	4.877126050	7.018801990	4.870412650
1	-2.474266750	2.848941910	-7.523713650
1	-7.493218640	2.523608720	2.105540090
1	2.051950000	3.224036670	7.231821010
1	7.072758960	3.506719160	-2.419796950
19	-0.489779900	4.747027400	-0.112638490

K@CG¹⁺:

7	0.061000000	-0.206000000	5.816000000
6	-0.026000000	-0.067000000	4.421000000
8	-1.110000000	-0.066000000	3.845000000
7	1.131000000	0.075000000	3.704000000
6	2.329000000	0.074000000	4.310000000
7	3.420000000	0.218000000	3.562000000
6	2.449000000	-0.089000000	5.734000000
6	1.293000000	-0.224000000	6.432000000
1	3.318000000	0.321000000	2.562000000
1	4.332000000	0.215000000	3.992000000
1	3.398000000	-0.109000000	6.250000000
1	1.305000000	-0.356000000	7.503000000
7	-4.648000000	-3.360000000	4.393000000
6	-3.440000000	-3.190000000	4.984000000
7	-2.453000000	-2.978000000	4.163000000
6	-3.067000000	-3.029000000	2.914000000
6	-2.512000000	-2.896000000	1.601000000
8	-1.342000000	-2.686000000	1.303000000
7	-3.462000000	-3.041000000	0.586000000
6	-4.803000000	-3.288000000	0.823000000
7	-5.594000000	-3.407000000	-0.232000000
7	-5.334000000	-3.415000000	2.050000000
6	-4.419000000	-3.275000000	3.049000000
1	-3.423000000	-3.268000000	6.061000000
1	-3.129000000	-2.944000000	-0.364000000
1	-5.213000000	-3.314000000	-1.164000000
1	-6.572000000	-3.613000000	-0.092000000
7	-0.146000000	0.160000000	-6.184000000
6	-0.034000000	0.213000000	-4.786000000
8	1.060000000	0.264000000	-4.233000000
7	-1.180000000	0.219000000	-4.038000000
6	-2.388000000	0.164000000	-4.620000000
7	-3.467000000	0.183000000	-3.842000000
6	-2.531000000	0.080000000	-6.049000000
6	-1.385000000	0.083000000	-6.777000000
1	-3.346000000	0.227000000	-2.839000000
1	-4.386000000	0.139000000	-4.253000000
1	-3.488000000	0.009000000	-6.545000000
1	-1.404000000	0.021000000	-7.854000000
7	4.772000000	-2.797000000	-5.027000000
6	3.558000000	-2.599000000	-5.596000000
7	2.574000000	-2.461000000	-4.757000000
6	3.197000000	-2.585000000	-3.518000000
6	2.641000000	-2.544000000	-2.199000000
8	1.463000000	-2.384000000	-1.895000000
7	3.597000000	-2.718000000	-1.193000000
6	4.946000000	-2.916000000	-1.449000000
7	5.751000000	-3.062000000	-0.405000000
7	5.474000000	-2.967000000	-2.685000000
6	4.553000000	-2.794000000	-3.674000000
1	3.529000000	-2.600000000	-6.675000000
1	3.258000000	-2.682000000	-0.240000000
1	5.376000000	-3.031000000	0.533000000
1	6.736000000	-3.220000000	-0.561000000

7	-6.031000000	-0.165000000	0.028000000
6	-4.632000000	-0.043000000	0.049000000
8	-3.981000000	0.022000000	-0.990000000
7	-3.998000000	0.009000000	1.261000000
6	-4.688000000	-0.065000000	2.409000000
7	-4.021000000	0.003000000	3.558000000
6	-6.118000000	-0.219000000	2.417000000
6	-6.733000000	-0.261000000	1.208000000
1	-3.016000000	0.102000000	3.530000000
1	-4.516000000	-0.053000000	4.435000000
1	-6.702000000	-0.301000000	3.323000000
1	-7.802000000	-0.375000000	1.135000000
7	-4.608000000	-3.132000000	-4.945000000
6	-5.205000000	-3.022000000	-3.731000000
7	-4.389000000	-2.881000000	-2.728000000
6	-3.137000000	-2.907000000	-3.333000000
6	-1.830000000	-2.809000000	-2.756000000
8	-1.544000000	-2.684000000	-1.570000000
7	-0.805000000	-2.872000000	-3.701000000
6	-1.028000000	-3.025000000	-5.058000000
7	0.040000000	-3.059000000	-5.840000000
7	-2.249000000	-3.133000000	-5.611000000
6	-3.261000000	-3.063000000	-4.701000000
1	-6.284000000	-3.081000000	-3.714000000
1	0.140000000	-2.782000000	-3.352000000
1	0.965000000	-2.969000000	-5.440000000
1	-0.080000000	-3.190000000	-6.834000000
7	6.031000000	0.346000000	-0.338000000
6	4.628000000	0.366000000	-0.323000000
8	4.001000000	0.363000000	0.733000000
7	3.962000000	0.399000000	-1.518000000
6	4.631000000	0.393000000	-2.682000000
7	3.934000000	0.438000000	-3.815000000
6	6.068000000	0.322000000	-2.724000000
6	6.712000000	0.301000000	-1.530000000
1	2.925000000	0.466000000	-3.765000000
1	4.410000000	0.424000000	-4.702000000
1	6.632000000	0.284000000	-3.645000000
1	7.786000000	0.239000000	-1.464000000
7	4.762000000	-3.165000000	4.295000000
6	5.344000000	-2.946000000	3.090000000
7	4.515000000	-2.749000000	2.108000000
6	3.272000000	-2.863000000	2.721000000
6	1.957000000	-2.777000000	2.161000000
8	1.663000000	-2.562000000	0.990000000
7	0.945000000	-2.979000000	3.105000000
6	1.187000000	-3.238000000	4.443000000
7	0.131000000	-3.409000000	5.226000000
7	2.417000000	-3.324000000	4.977000000
6	3.414000000	-3.129000000	4.069000000
1	6.424000000	-2.980000000	3.067000000
1	-0.007000000	-2.917000000	2.775000000
1	-0.802000000	-3.344000000	4.840000000
1	0.272000000	-3.622000000	6.201000000
19	0.118156470	-1.364916940	-0.310868660

1	-0.772083400	-0.291962710	6.362426990
1	-5.525338940	-3.515478140	4.846985600
1	5.223354140	-3.320668300	5.168452770
1	6.537821510	0.364610700	0.523850100
1	5.646173490	-2.919805680	-5.496829200
1	0.677547360	0.178267080	-6.750953310
1	-5.056983590	-3.240655060	-5.831909140
1	-6.517701500	-0.182139610	-0.845400190

K@TG¹:

7	-4.445000000	8.389000000	-3.596000000
6	-3.071000000	8.419000000	-3.364000000
8	-2.255000000	8.813000000	-4.182000000
7	-2.632000000	7.996000000	-2.135000000
6	-3.438000000	7.621000000	-1.084000000
8	-2.909000000	7.359000000	-0.009000000
6	-4.874000000	7.598000000	-1.387000000
6	-5.908000000	7.191000000	-0.342000000
6	-5.316000000	7.975000000	-2.616000000
1	-1.632000000	7.959000000	-1.993000000
1	-5.427000000	6.698000000	0.502000000
1	-6.422000000	8.076000000	0.034000000
1	-6.644000000	6.507000000	-0.768000000
1	-6.368000000	7.943000000	-2.863000000
7	-2.083000000	4.332000000	-6.097000000
6	-3.213000000	4.058000000	-5.372000000
7	-3.029000000	4.006000000	-4.080000000
6	-1.652000000	4.203000000	-3.948000000
6	-0.800000000	4.252000000	-2.797000000
8	-1.116000000	4.171000000	-1.621000000
7	0.537000000	4.422000000	-3.086000000
6	1.016000000	4.539000000	-4.344000000
7	2.311000000	4.618000000	-4.475000000
7	0.265000000	4.515000000	-5.440000000
6	-1.063000000	4.351000000	-5.181000000
1	-4.179000000	3.917000000	-5.826000000
1	1.141000000	4.489000000	-2.285000000
1	2.937000000	4.564000000	-3.674000000
1	2.636000000	4.604000000	-5.425000000
7	-4.442000000	8.318000000	4.516000000
6	-4.169000000	8.222000000	3.151000000
8	-4.989000000	8.449000000	2.276000000
7	-2.894000000	7.867000000	2.789000000
6	-1.847000000	7.657000000	3.655000000
8	-0.732000000	7.449000000	3.187000000
6	-2.202000000	7.724000000	5.077000000
6	-1.178000000	7.445000000	6.170000000
6	-3.469000000	8.049000000	5.449000000
1	-2.719000000	7.755000000	1.799000000
1	-0.861000000	8.379000000	6.634000000
1	-1.593000000	6.782000000	6.932000000
1	-0.297000000	6.963000000	5.749000000
1	-3.744000000	8.093000000	6.494000000
7	-6.599000000	4.029000000	2.281000000
6	-5.880000000	3.917000000	3.441000000

7	-4.583000000	3.958000000	3.284000000
6	-4.440000000	4.039000000	1.894000000
6	-3.282000000	4.113000000	1.053000000
8	-2.110000000	4.157000000	1.389000000
7	-3.561000000	4.145000000	-0.297000000
6	-4.814000000	4.121000000	-0.799000000
7	-4.935000000	4.102000000	-2.098000000
7	-5.917000000	4.064000000	-0.061000000
6	-5.668000000	4.030000000	1.278000000
1	-6.350000000	3.826000000	4.406000000
1	-2.760000000	4.211000000	-0.899000000
1	-4.131000000	4.079000000	-2.723000000
1	-5.878000000	4.015000000	-2.429000000
7	3.844000000	8.037000000	-3.769000000
6	3.684000000	7.865000000	-2.395000000
8	4.609000000	7.870000000	-1.604000000
7	2.409000000	7.692000000	-1.916000000
6	1.271000000	7.667000000	-2.690000000
8	0.184000000	7.569000000	-2.130000000
6	1.502000000	7.785000000	-4.134000000
6	0.361000000	7.655000000	-5.135000000
6	2.760000000	7.978000000	-4.613000000
1	2.298000000	7.618000000	-0.913000000
1	-0.474000000	7.115000000	-4.687000000
1	0.018000000	8.645000000	-5.435000000
1	0.679000000	7.102000000	-6.021000000
1	2.931000000	8.095000000	-5.675000000
7	6.236000000	4.772000000	-1.533000000
6	5.520000000	4.484000000	-2.664000000
7	4.227000000	4.439000000	-2.493000000
6	4.092000000	4.606000000	-1.111000000
6	2.941000000	4.618000000	-0.259000000
8	1.765000000	4.581000000	-0.585000000
7	3.232000000	4.687000000	1.087000000
6	4.488000000	4.781000000	1.576000000
7	4.615000000	4.809000000	2.875000000
7	5.583000000	4.819000000	0.824000000
6	5.324000000	4.729000000	-0.513000000
1	5.991000000	4.334000000	-3.619000000
1	2.436000000	4.729000000	1.697000000
1	3.822000000	4.696000000	3.505000000
1	5.564000000	4.816000000	3.199000000
7	3.822000000	8.617000000	4.716000000
6	2.468000000	8.347000000	4.523000000
8	1.632000000	8.425000000	5.408000000
7	2.072000000	7.993000000	3.254000000
6	2.897000000	7.901000000	2.155000000
8	2.402000000	7.657000000	1.058000000
6	4.319000000	8.127000000	2.440000000
6	5.385000000	7.954000000	1.369000000
6	4.722000000	8.474000000	3.689000000
1	1.087000000	7.803000000	3.118000000
1	6.292000000	7.503000000	1.776000000
1	5.010000000	7.285000000	0.602000000
1	5.619000000	8.911000000	0.905000000

1	5.769000000	8.635000000	3.907000000
7	1.726000000	4.504000000	6.886000000
6	2.886000000	4.457000000	6.160000000
7	2.719000000	4.473000000	4.864000000
6	1.326000000	4.459000000	4.729000000
6	0.475000000	4.450000000	3.577000000
8	0.798000000	4.501000000	2.401000000
7	-0.872000000	4.381000000	3.864000000
6	-1.365000000	4.345000000	5.121000000
7	-2.658000000	4.231000000	5.247000000
7	-0.618000000	4.363000000	6.220000000
6	0.719000000	4.424000000	5.962000000
1	3.854000000	4.427000000	6.630000000
1	-1.480000000	4.383000000	3.065000000
1	-3.279000000	4.147000000	4.444000000
1	-2.980000000	4.139000000	6.193000000
1	4.755538610	8.204852670	-4.144396920
1	-4.801757190	8.672096160	-4.486270110
1	-5.356546720	8.585729680	4.819191540
1	4.141918210	8.918749930	5.614108750
1	1.634053570	4.580418560	7.878827310
1	-7.592318580	4.095799400	2.186893460
1	-2.016526530	4.485266420	-7.082946590
1	7.213782620	4.970782260	-1.466466160
19	-0.127023410	6.015675900	0.360834330

K@UG¹:

7	1.535814000	-6.421984000	-0.775097000
6	0.166905000	-6.336826000	-0.854376000
7	-0.277175000	-5.178721000	-1.257984000
6	0.881719000	-4.418754000	-1.427333000
6	1.056680000	-3.036712000	-1.780387000
8	0.194088000	-2.192503000	-2.014071000
7	2.378048000	-2.633876000	-1.810229000
6	3.413263000	-3.461786000	-1.514115000
7	4.614260000	-2.952069000	-1.478832000
7	3.295287000	-4.744191000	-1.171760000
6	1.996641000	-5.173360000	-1.141343000
1	-0.489067000	-7.163117000	-0.618506000
1	2.554003000	-1.663845000	-2.022071000
1	4.768203000	-1.966760000	-1.663766000
1	5.381189000	-3.512138000	-1.136144000
7	-1.910299000	-5.190071000	2.561195000
6	-2.458859000	-3.943170000	2.253525000
8	-3.643765000	-3.656111000	2.437914000
7	-1.596971000	-2.994175000	1.755650000
6	-0.245619000	-3.149761000	1.593903000
8	0.416245000	-2.239824000	1.107166000
6	0.274422000	-4.422809000	2.041559000
6	-0.549991000	-5.396540000	2.511852000
1	-1.977796000	-2.089384000	1.530043000
1	1.337105000	-4.588880000	1.987545000
1	-0.155172000	-6.346436000	2.856205000
7	-6.629799000	-1.573345000	-1.293373000
6	-6.596343000	-0.201466000	-1.266298000

7	-5.402537000	0.306203000	-1.437090000
6	-4.579114000	-0.818339000	-1.573457000
6	-3.155562000	-0.949628000	-1.752110000
8	-2.305231000	-0.063357000	-1.827618000
7	-2.723961000	-2.259736000	-1.828452000
6	-3.564182000	-3.324687000	-1.752556000
7	-3.047971000	-4.514544000	-1.828925000
7	-4.879581000	-3.248849000	-1.580149000
6	-5.330911000	-1.966047000	-1.494631000
1	-7.484680000	0.400554000	-1.125163000
1	-1.742333000	-2.412792000	-1.992958000
1	-2.051117000	-4.665547000	-1.841994000
1	-3.699889000	-5.293360000	-1.850347000
7	-5.740783000	1.574466000	2.255667000
6	-4.574556000	2.285539000	1.933143000
8	-4.497525000	3.513453000	1.923676000
7	-3.463117000	1.547226000	1.588324000
6	-3.412693000	0.182904000	1.484875000
8	-2.360345000	-0.360588000	1.160413000
6	-4.660013000	-0.490276000	1.780232000
6	-5.769225000	0.198985000	2.161191000
1	-2.597300000	2.039322000	1.461649000
1	-4.694433000	-1.564001000	1.704454000
1	-6.683448000	-0.327871000	2.417441000
7	-1.531289000	6.629692000	-0.815222000
6	-0.157486000	6.606492000	-0.864081000
7	0.350437000	5.436398000	-1.151334000
6	-0.774854000	4.614657000	-1.276121000
6	-0.896849000	3.207500000	-1.538295000
8	0.000914000	2.382038000	-1.700157000
7	-2.203876000	2.760377000	-1.583253000
6	-3.274975000	3.563966000	-1.359601000
7	-4.467766000	3.039498000	-1.412091000
7	-3.207665000	4.866798000	-1.100209000
6	-1.925850000	5.339540000	-1.071804000
1	0.449542000	7.485917000	-0.689255000
1	-2.351018000	1.784645000	-1.795292000
1	-4.606911000	2.050257000	-1.584906000
1	-5.264303000	3.626673000	-1.234031000
7	1.765048000	5.260169000	2.343567000
6	2.369024000	4.036312000	2.024716000
8	3.587012000	3.837552000	2.063616000
7	1.527514000	3.004394000	1.669618000
6	0.154554000	3.051952000	1.661556000
8	-0.492983000	2.048348000	1.371096000
6	-0.406134000	4.329453000	2.030850000
6	0.390931000	5.381311000	2.358000000
1	1.948128000	2.101923000	1.512710000
1	-1.482234000	4.429169000	2.070200000
1	-0.049764000	6.320449000	2.665859000
7	6.729477000	1.589855000	-0.840740000
6	6.646429000	0.234117000	-1.043685000
7	5.460248000	-0.189742000	-1.374260000
6	4.687482000	0.973117000	-1.390948000
6	3.281410000	1.156572000	-1.623598000

8	2.423423000	0.297726000	-1.831263000
7	2.884583000	2.478545000	-1.576237000
6	3.731683000	3.508058000	-1.306959000
7	3.212745000	4.706798000	-1.251652000
7	5.039181000	3.380968000	-1.056953000
6	5.464141000	2.077760000	-1.107972000
1	7.496718000	-0.425781000	-0.935348000
1	1.906759000	2.660252000	-1.738553000
1	2.218350000	4.855481000	-1.381122000
1	3.796467000	5.495374000	-1.020635000
7	5.402994000	-2.200293000	2.074400000
6	4.117206000	-2.683201000	1.803605000
8	3.819532000	-3.880731000	1.817379000
7	3.143242000	-1.746099000	1.536257000
6	3.306628000	-0.385776000	1.551984000
8	2.366215000	0.341107000	1.243099000
6	4.627103000	0.051432000	1.945337000
6	5.623253000	-0.843354000	2.199077000
1	2.207749000	-2.074645000	1.358317000
1	4.803826000	1.113109000	2.040906000
1	6.597877000	-0.494867000	2.514291000
1	-6.556641000	2.068596000	2.556015000
1	-2.118308000	7.418228000	-0.631865000
1	2.334947000	6.052198000	2.562435000
1	7.534134000	2.112755000	-0.559489000
1	6.164289000	-2.840396000	2.177837000
1	2.080910000	-7.217124000	-0.509350000
1	-2.514118000	-5.943654000	2.821032000
1	-7.431367000	-2.161993000	-1.188571000
19	0.177836000	-0.178847000	-0.211992000