Electronic Supplementary material

Title: Sandwiches of N-doped Diamondoid and Benzene via Lone Pair-cation and Cation-pi Interaction: A DFT study

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Journal: New Journal of Chemistry

Date: 05/10/2017

Supplementary Table S1: Cartesian coordinates of the complexes are provided below:

Complexes	Cartesian Coordinates			
N-Ada@Li$^+$	C	0.63493200	1.39725000	-0.38781400
	C	0.63376300	-1.03465100	-1.01600100
	C	0.63416400	-0.36280700	1.40382800
	C	-0.90445200	1.36268600	-0.37851300
	C	-0.90534800	-1.00889900	-0.99038100
	C	-0.90501400	-0.35321600	1.36910100
	C	1.15002000	0.36465800	-1.41280500
	C	1.15033000	1.04083800	1.02241700
	C	1.14952400	-1.40656200	0.39015500
	H	0.95799800	2.40627800	-0.66821400
	H	0.95640500	-1.78199600	-1.74987100
	H	0.95700800	-0.62472600	2.41787500
	H	-1.30331200	1.61315300	-1.36983400
	H	-1.30394000	2.08899000	0.34085000
	H	-1.30466500	-1.99241300	-0.71143700
	H	-1.30490400	-0.74898100	-1.97896800
	H	-1.30376800	0.38004500	2.08174900
	H	-1.30488000	-1.33930200	1.63789300
	H	0.81198300	0.62594600	-2.42396200
	H	2.24549000	0.36939700	-1.43428300
	H	2.24578900	1.05643800	1.03803500
	H	0.81221700	1.78603800	1.75410300
	H	0.81054900	-2.41249800	0.66982000
	H	2.24494800	-1.42850300	0.39621000
	N	-1.42345500	0.00049900	0.00009700
	Li	-3.36008100	0.00095100	-0.00018700

N-Ada@Na$^+$	C	0.99064300	0.67583500	-1.28266000
	C	0.99020800	-1.44901000	0.05590700
	C	0.99102300	0.77278000	1.22662300
	C	-0.54914400	0.65688200	-1.24608400
	C	-0.54962500	-1.40754600	0.05448300
	C	-0.54887400	0.75103700	1.19189100
	C	1.50696600	-0.77789200	-1.23433500
	C	1.50750200	1.45780200	-0.05640300
	C	1.50728400	-0.68034600	1.29041300
	H	1.31368100	1.16416400	-2.20948000
	H	1.31324200	-2.49583600	0.09635700
	H	1.31407600	1.33109700	2.11301600
	H	-0.94790300	0.10860300	-2.10942800
	H	-0.94742100	1.67919400	-1.28158500
	H	-0.94791900	-1.88092500	0.96126200
	H	-0.94813700	-1.94944400	-0.81299000
	H	-0.94719600	1.77305000	1.14854500
	H	-0.94760000	0.27114500	2.09508700
	H	1.16728300	-1.33443800	-2.11771300
	H	2.60263100	-0.79067900	-1.25432300
	H	2.60316900	1.48110400	-0.05755700
	H	1.16809700	2.50118900	-0.09671200
	H	1.16794300	-1.16710000	2.21420000
	H	2.60295800	-0.69150900	1.31092700
	N	-1.06635800	0.00020700	0.00017300
	Na	-3.37984400	0.00015300	0.00001600
N-Ada@K$^+$	C	1.36462900	-0.53752900	1.34730900
	C	1.36502700	1.43525800	-0.20804000
	C	1.36575200	-0.89780200	-1.13897900
	C	-0.17655500	-0.51941400	1.30308400
	C	-0.17583900	1.38847200	-0.20144800
	C	-0.17539700	-0.86920900	-1.10158600
	C	1.88256200	0.90286100	1.14516300
	C	1.88231000	-1.44339500	0.20947300
	C	1.88283600	0.54077900	-1.35434700
	H	1.68877700	-0.92577100	2.32019400
	H	1.68959800	2.47185100	-0.35795300
	H	1.69034800	-1.54621800	-1.96147300
	H	-0.57555800	0.11606600	2.10517800
	H	-0.57548900	-1.53238000	1.44842200
	H	-0.57419500	1.76617100	-1.15278500
	H	-0.57474800	2.02027200	0.60360600
	H	-0.57290100	-1.88203500	-0.95137900
	H	-0.57523600	-0.48963000	-2.05158000
	H	1.54306100	1.54950200	1.96524400
	H	2.97849400	0.91702500	1.16371300
	H	2.97823000	-1.46698700	0.21336200
	H	1.54205900	-2.47676200	0.35857600
	H	1.54388800	0.92812200	-2.32439700
	H	2.97884300	0.55005400	-1.37560100
	N	-0.68912600	-0.00026300	-0.00019400
	K	-3.45543400	0.00012800	-0.00029100
N-Ada-Ben@Li$^+$	C	-2.50669900	-1.01445000	-1.03249800
	C	-2.49085800	1.40563200	-0.36160500
	C	-2.49558100	-0.38526000	1.39848100
	C	-0.96705400	-0.99491700	-1.00888300
	C	-0.95160700	1.35806900	-0.35640700
	C	-0.95608600	-0.38344100	1.35491900
	C	-3.01700000	0.39459700	-1.40235600
	C	-3.02161100	-1.40725300	0.36834400
	C	-3.00581200	1.02746200	1.04310300
	H	-2.83697600	-1.74674300	-1.77849100
	H	-2.80973100	2.42142400	-0.62307300
	H	-2.81775100	-0.66317600	2.40882800
	H	-0.56775700	-0.71975400	-1.99304900
	H	-0.57064800	-1.98471600	-0.75006300

	H	-0.54436000	2.06857200	0.37383900
	H	-0.55233500	1.62414300	-1.34311700
	H	-0.56045600	-1.37594500	1.60449900
	H	-0.54861800	0.33308100	2.07911900
	H	-2.67953900	0.67167600	-2.40972700
	H	-4.11280100	0.40674900	-1.42048700
	H	-4.11748300	-1.42311100	0.37733400
	H	-2.68714000	-2.41998600	0.62905700
	H	-2.66001700	1.75746700	1.78675700
	H	-4.10144400	1.04977900	1.06279900
	N	-0.44166800	-0.00965200	-0.00506100
	Li	1.52828900	-0.01661400	-0.00335100
	C	3.49209800	0.96518900	1.02240900
	C	3.49121800	1.36910100	-0.32213600
	C	3.50123000	0.40657800	-1.34407500
	C	3.51256500	-0.95973300	-1.02138600
	C	3.51373200	-1.36362300	0.32323100
	C	3.50370600	-0.40109700	1.34518300
	H	3.49209200	1.70951700	1.81262100
	H	3.48989900	2.42561500	-0.57144400
	H	3.50812000	0.71869300	-2.38376600
	H	3.52779300	-1.70392800	-1.81155100
	H	3.53067200	-2.42002600	0.57255900
	H	3.51184400	-0.71305500	2.38489500
N-Ada-Ben@Na^+	C	2.90501300	1.18830000	0.83373900
	C	2.89872800	0.13706500	-1.44721400
	C	2.92298000	-1.31318100	0.60377500
	C	1.36495900	1.14030700	0.81799800
	C	1.35863000	0.12078500	-1.39403300
	C	1.38202100	-1.28518600	0.59472000
	C	3.41202000	1.33332000	-0.61678900
	C	3.43685000	-0.12549800	1.44573200
	C	3.42998800	-1.18317300	-0.84850200
	H	3.22627700	2.04626800	1.43624100
	H	3.21524400	0.23520700	-2.49241700
	H	3.25688800	-2.26212500	1.04014100
	H	0.95532000	2.06473300	0.39055400
	H	0.97326300	1.04023400	1.83850100
	H	0.96229900	-0.71949500	-1.97863600
	H	0.94911900	1.04721300	-1.81702400
	H	0.98901800	-1.37900000	1.61530200
	H	0.98532100	-2.12152200	0.00464500
	H	3.06163700	2.27887400	-1.05157800
	H	4.50764400	1.36417700	-0.63344000
	H	4.53288700	-0.11882300	1.46187500
	H	3.10520200	-0.22318400	2.48793900
	H	3.09279500	-2.03840400	-1.44888800
	H	4.52594500	-1.19426900	-0.86900900
	N	0.85348300	-0.01199400	0.00934400
	C	-3.96518100	-1.16711600	-0.77628400
	C	-3.94951700	0.08745600	-1.40490600
	C	-3.94616800	1.25931200	-0.63295500
	C	-3.95728100	1.17665400	0.76785800
	C	-3.97302200	-0.07789800	1.39658700
	C	-3.97671100	-1.24980600	0.62455500
	H	-3.99460500	-2.07348200	-1.37381200
	H	-3.96722600	0.15150200	-2.48885600
	H	-3.96076400	2.23001800	-1.11967700
	H	-3.98098200	2.08344800	1.36496200
	H	-4.00843300	-0.14150200	2.48014700
	H	-4.01519200	-2.22006900	1.11080400
	Na	-1.49508000	-0.01944400	0.01737600
N-Ada-Ben@K^+	C	3.37036800	-1.02181500	1.02638800
	C	3.34891200	1.40627400	0.38002200
	C	3.36633400	-0.36866900	-1.39702000
	C	1.82832900	-1.00094600	0.98984300

	C	1.80721100	1.34602700	0.36402200
	C	1.82411100	-0.36801900	-1.35307200
	C	3.87590800	0.38588200	1.40933100
	C	3.89399100	-1.39739900	-0.37646500
	C	3.87196800	1.04226000	-1.02642500
	H	3.70129800	-1.75912100	1.76786300
	H	3.66577400	2.42027300	0.65254800
	H	3.69536400	-0.63672000	-2.40795800
	H	1.42563100	-0.73728200	1.97687400
	H	1.43540600	-1.99098600	0.72159800
	H	1.40444300	2.06448900	-0.36283100
	H	1.40102100	1.60846400	1.35013000
	H	1.43013000	-1.35793900	-1.62049000
	H	1.42123500	0.35477900	-2.07571200
	H	3.53565900	0.65197900	2.41873800
	H	4.97196700	0.40260200	1.43022700
	H	4.99050800	-1.40769000	-0.38065300
	H	3.56643800	-2.40986200	-0.64720200
	H	3.52918200	1.77796000	-1.76602000
	H	4.96803200	1.06462900	-1.03928000
	N	1.30851300	-0.01189800	0.00003800
	C	-4.49731500	0.98862900	-0.99174900
	C	-4.47844700	1.36441000	0.35874300
	C	-4.47621400	0.38291800	1.35923700
	C	-4.49446300	-0.97460300	1.00953200
	C	-4.51120800	-1.35040900	-0.34095500
	C	-4.51269300	-0.36885900	-1.34140600
	H	-4.53336700	1.74908300	-1.76660600
	H	-4.49960300	2.41613400	0.62957300
	H	-4.49641500	0.67451400	2.40533400
	H	-4.52684600	-1.73442400	1.78516500
	H	-4.55878600	-2.40142100	-0.61120700
	H	-4.56020900	-0.65983000	-2.38683800
	K	-1.49616900	-0.02107500	-0.02598300
N-Di@Li$^+$	C	-0.38464100	1.43238000	-0.26652100
	C	0.16313500	0.48158400	-1.36179800
	C	0.16224500	0.93924400	1.09743100
	C	-0.38371500	-0.94716000	-1.10678300
	C	-0.38457600	-0.48547200	1.37370600
	C	0.16304000	-1.41991300	0.26441100
	C	-2.44319300	-0.00043400	-0.00031400
	C	-1.92487100	1.42731800	-0.26467300
	C	1.69863400	0.47061400	-1.32915700
	C	1.69789000	0.91649600	1.07214400
	C	-1.92403900	-0.94298000	-1.10390700
	C	-1.92495400	-0.48475600	1.36778700
	C	1.69820800	-1.38686600	0.25733300
	H	-0.02113700	2.45263200	-0.45552400
	H	-0.15716600	0.83169700	-2.35171900
	H	-0.15848400	1.62140500	1.89543400
	H	-0.01989000	-1.62132200	-1.89540200
	H	-0.02183600	-0.83162700	2.35217700
	H	-0.15795000	-2.45212600	0.45578000
	H	-3.53886300	-0.00048100	-0.00074700
	H	-2.29784800	1.79744000	-1.22796300
	H	-2.29600000	2.11643800	0.50443900
	H	2.09595200	1.47772600	-1.51153000
	H	2.09667700	-0.19662100	-2.10479200
	H	2.09516400	0.57178200	2.03588000
	H	2.09562900	1.92194400	0.88164100
	H	-2.29688000	-1.96214900	-0.94170600
	H	-2.29541900	-0.62235800	-2.08540200
	H	-2.29857800	0.16476000	2.16927700
	H	-2.29631900	-1.49530900	1.57962800
	H	2.09482800	-2.04821000	-0.52417100
	H	2.09635800	-1.72590100	1.22266000

	N	2.22071400	0.00021300	0.00018500
	Li	4.15259700	-0.00051300	0.00093200
N-Di@Na$^+$	C	0.71051300	-1.42646300	-0.29670600
	C	0.16221300	-0.45241100	-1.37140300
	C	0.16261000	-0.96171000	1.07732200
	C	0.70955700	0.97008100	-1.08666300
	C	0.71018000	0.45635300	1.38318800
	C	0.16189700	1.41429200	0.29423200
	C	2.76832100	0.00032800	0.00002400
	C	2.25030200	-1.42151000	-0.29510800
	C	-1.37418600	-0.44060000	-1.33412200
	C	-1.37376100	-0.93564700	1.04731000
	C	2.24934500	0.96719100	-1.08306700
	C	2.25013200	0.45515000	1.37874500
	C	-1.37467300	1.37516500	0.28505600
	H	0.34639000	-2.44237900	-0.50784100
	H	0.48355700	-0.78133200	-2.36850900
	H	0.48367700	-1.66074300	1.86088800
	H	0.34539500	1.66082600	-1.86102800
	H	0.34673600	0.78125600	2.36891500
	H	0.48296500	2.44234000	0.50786200
	H	3.86410300	0.00037300	-0.00040600
	H	2.62351100	-1.76972600	-1.26654500
	H	2.62222200	-2.12671400	0.45906400
	H	-1.76979100	-1.44398500	-1.54040400
	H	-1.77059400	0.24192300	-2.09755400
	H	-1.77084700	-0.61305800	2.01898200
	H	-1.77025300	-1.93771300	0.83640200
	H	2.62193700	1.98267800	-0.89777000
	H	2.62219100	0.66805700	-2.07090100
	H	2.62237100	-0.21274600	2.16597700
	H	2.62254300	1.46030700	1.61393900
	H	-1.77026900	2.05477300	-0.48143700
	H	-1.77211000	1.69469600	1.25752300
	N	-1.89483900	-0.00035500	-0.00065000
	Na	-4.20677800	0.00021100	0.00132300
N-Di@K$^+$	C	-1.05316700	-0.40775300	1.39755500
	C	-0.50472700	0.99897700	1.04399200
	C	-0.50486800	-1.40368100	0.34309300
	C	-1.05263100	1.41459300	-0.34581100
	C	-1.05259700	-1.00674600	-1.05213400
	C	-0.50387000	0.40455600	-1.38656500
	C	-3.11167300	0.00007000	-0.00079800
	C	-2.59302300	-0.40638100	1.39290800
	C	1.03274100	0.96794700	1.01183600
	C	1.03276700	-1.35925200	0.33365100
	C	-2.59272300	1.41011100	-0.34570400
	C	-2.59273300	-1.00387500	-1.04928400
	C	1.03351200	0.39202600	-1.34189600
	H	-0.68973500	-0.69828400	2.39404800
	H	-0.82789300	1.72493200	1.80220400
	H	-0.82759600	-2.42345300	0.59213800
	H	-0.68839000	2.42267700	-0.59197700
	H	-0.68872500	-1.72450500	-1.80185300
	H	-0.82536600	0.69850200	-2.39470600
	H	-4.20763100	0.00022400	-0.00098900
	H	-2.96661000	0.28880300	2.15575000
	H	-2.96635400	-1.40279100	1.66194400
	H	1.42896200	0.68149000	1.99573300
	H	1.42918400	1.96304900	0.76701800
	H	1.43058200	-2.06768100	-0.40620100
	H	1.42782600	-1.64509100	1.31829700
	H	-2.96486200	1.72213700	-1.32998200
	H	-2.96654800	2.14212100	0.38174000
	H	-2.96520800	-2.01226700	-0.82782500
	H	-2.96563200	-0.73979800	-2.04716700

	H	1.43016200	1.38772900	-1.58385800
	H	1.43097800	-0.31625800	-2.08201400
	N	1.55019900	0.00005200	0.00154900
	K	4.31049600	-0.00028700	-0.00095800
N-Di-Ben@Li$^+$	C	2.12731600	-0.38649800	1.40380600
	C	1.57581500	-1.39800900	0.36643400
	C	1.57760800	1.01446500	1.02917800
	C	2.11959100	-1.02337400	-1.03592400
	C	2.12137500	1.40966300	-0.36763800
	C	1.57033400	0.38310000	-1.39034200
	C	4.18155000	0.00070000	-0.00609700
	C	3.66749100	-0.38527600	1.39469100
	C	0.03952100	-1.36098600	0.36005400
	C	0.04178500	0.98685700	1.00700600
	C	3.65920600	-1.01950900	-1.03766700
	C	3.66146400	1.40551900	-0.37038200
	C	0.03454900	0.37290600	-1.34904500
	H	1.76690800	-0.66177400	2.40559600
	H	1.89825000	-2.41401300	0.63013000
	H	1.90127400	1.75157700	1.77605100
	H	1.75311800	-1.75171400	-1.77380700
	H	1.75640100	2.41365600	-0.62839300
	H	1.88915500	0.66114700	-2.40369200
	H	5.27745100	0.00047900	-0.01011500
	H	4.04093500	-1.37784100	1.67719800
	H	4.04238600	0.32072000	2.14669000
	H	-0.35675000	-1.62970000	1.34768400
	H	-0.36119500	-2.07742500	-0.36847600
	H	-0.35824600	1.97545400	0.74753100
	H	-0.35427100	0.71233300	1.99294900
	H	4.02894000	-0.77040200	-2.04041300
	H	4.03308900	-2.02411400	-0.80206000
	H	4.03626200	2.14870600	0.34504400
	H	4.03076400	1.70384100	-1.35996100
	H	-0.36597100	-0.34698000	-2.07438400
	H	-0.36536900	1.36309800	-1.60253900
	N	-0.48201600	-0.00064100	0.00715400
	Li	-2.44870400	-0.00034200	0.00340700
	C	-4.42111200	-1.04957700	-0.93439900
	C	-4.42586800	-1.33211200	0.44057900
	C	-4.42749500	-0.28218100	1.37283300
	C	-4.42570400	1.05011400	0.93014400
	C	-4.42210400	1.33259100	-0.44485600
	C	-4.42027100	0.28275000	-1.37709200
	H	-4.42609500	-1.86111100	-1.65537000
	H	-4.43360700	-2.36215100	0.78301900
	H	-4.43780700	-0.50047000	2.43615100
	H	-4.43326400	1.86158700	1.65111600
	H	-4.42835900	2.36259700	-0.78753300
	H	-4.42408200	0.50116000	-2.44041800
N-Di-Ben@Na$^+$	C	2.50193300	-1.10814500	-0.94437400
	C	1.95348200	0.26318300	-1.41756700
	C	1.95980800	-1.36037000	0.48586400
	C	2.50745400	1.37267600	-0.48698400
	C	2.51462400	-0.26412800	1.43191300
	C	1.96553600	1.10011200	0.93975600
	C	4.56669600	-0.00270600	-0.00981200
	C	4.04201300	-1.10703900	-0.94868300
	C	0.41739300	0.25858800	-1.36975600
	C	0.42298100	-1.31831900	0.47767300
	C	4.04711900	1.36624700	-0.49293100
	C	4.05449000	-0.26542300	1.42021000
	C	0.42821300	1.06978300	0.91972000
	H	2.13335700	-1.89697400	-1.61618000
	H	2.27163900	0.45333900	-2.45145200
	H	2.28159200	-2.35040300	0.83579100

	H	2.14246100	2.35085600	-0.83240700
	H	2.15528300	-0.45173700	2.45420300
	H	2.29221600	1.89846300	1.61955700
	H	5.66268800	-0.00382600	-0.01515700
	H	4.41001900	-0.94513200	-1.96996200
	H	4.41522400	-2.08830100	-0.62844200
	H	0.01592200	-0.52076100	-2.03085600
	H	0.02037600	1.22463100	-1.70855000
	H	0.02906200	-1.50234100	1.48593400
	H	0.02160900	-2.09510200	-0.18654600
	H	4.42486500	2.16709100	0.15569000
	H	4.41567400	1.57749200	-1.50499900
	H	4.42811300	-1.22995600	1.78703000
	H	4.43156100	0.50351900	2.10655900
	H	0.03027000	2.03482900	0.57891300
	H	0.03554700	0.88145000	1.92774100
	N	-0.09582300	0.00445900	0.01117200
	C	-4.91921200	1.28424300	-0.56013900
	C	-4.89496400	0.16067800	-1.40043600
	C	-4.88682700	-1.12891900	-0.84757900
	C	-4.90218600	-1.29473200	0.54571500
	C	-4.92611200	-0.17120500	1.38601300
	C	-4.93395700	1.11833300	0.83311100
	H	-4.95413800	2.28157200	-0.98844800
	H	-4.91085200	0.28910500	-2.47866000
	H	-4.89693600	-1.99851700	-1.49801500
	H	-4.92359600	-2.29274100	0.97334100
	H	-4.96640800	-0.30011700	2.46351300
	H	-4.97835600	1.98735800	1.48285300
	Na	-2.43884700	0.01435100	0.01727800
N-Di-Ben@K⁺	C	2.92452200	1.44635400	0.17602900
	C	2.37525100	0.56585700	1.32852100
	C	2.37902800	0.86840700	-1.15554700
	C	2.92559100	-0.87443900	1.16370800
	C	2.92990900	-0.56939800	-1.33933300
	C	2.37999400	-1.43462700	-0.17546400
	C	4.98534800	0.00362900	0.00425500
	C	4.46440300	1.44403500	0.17845500
	C	0.83804600	0.54569700	1.28316200
	C	0.84135600	0.83856700	-1.12052900
	C	4.46537100	-0.86987200	1.16349700
	C	4.46978100	-0.56600400	-1.33249500
	C	0.84200100	-1.38914300	-0.17267000
	H	2.55876800	2.47610900	0.30087800
	H	2.69648200	0.97730700	2.29504700
	H	2.70261400	1.49942100	-1.99446200
	H	2.56072200	-1.49801500	1.99308100
	H	2.56835100	-0.97628700	-2.29508000
	H	2.70440400	-2.47647000	-0.30189200
	H	6.08145100	0.00504300	0.00653800
	H	4.83506200	1.87173400	1.11890800
	H	4.83837400	2.08421000	-0.63098900
	H	0.43881700	1.56171700	1.40614900
	H	0.44088100	-0.07119000	2.10092100
	H	0.44607000	0.43641500	-2.06340300
	H	0.44215500	1.85459200	-0.99728000
	H	4.84065400	-1.89670200	1.06494100
	H	4.83558800	-0.48757200	2.12359400
	H	4.84341600	0.03474200	-2.17174800
	H	4.84441900	-1.58700000	-1.48092800
	H	0.44382300	-2.00540800	0.64509200
	H	0.44717000	-1.78980500	-1.11641000
	N	0.32514900	-0.00212000	-0.00391900
	C	-5.48192700	-0.76292900	1.17053100
	C	-5.45115300	0.63582600	1.25858900
	C	-5.43880000	1.41155600	0.09100900

	C	-5.45649700	0.78845200	-1.16465900
	C	-5.48730400	-0.61030500	-1.25262100
	C	-5.50117100	-1.38598300	-0.08505200
	H	-5.52553600	-1.36290700	2.07498700
	H	-5.47147800	1.11922700	2.23113100
	H	-5.45025700	2.49559900	0.15931400
	H	-5.48098000	1.38991900	-2.06883600
	H	-5.53505600	-1.09223700	-2.22491000
	H	-5.55935800	-2.46849800	-0.15301500
	K	-2.46553200	-0.03122000	-0.00581700
N-Tri@Li$^+$	C	0.60467300	-1.43689300	1.25676000
	C	1.50684400	-1.50676900	0.00000000
	C	0.60467300	-1.43689300	-1.25676000
	C	-0.42407800	-2.58393600	-1.25709300
	C	-1.31136700	-2.48800000	0.00000000
	C	-0.42407800	-2.58393600	1.25709300
	H	1.23135800	-1.50337300	2.15666700
	H	2.04945300	-2.46060900	0.00000000
	H	1.23135800	-1.50337300	-2.15666700
	H	-1.04086700	-2.53645900	-2.16421600
	H	0.09528000	-3.54989500	-1.27799900
	H	-2.04288000	-3.30420800	0.00000000
	H	-1.04086700	-2.53645900	2.16421600
	H	0.09528000	-3.54989500	1.27799900
	C	-0.12801500	-0.07482700	1.25862400
	C	-1.04095600	0.02090900	0.00000000
	C	-2.05756200	-1.13709700	0.00000000
	C	-0.12801500	-0.07482700	-1.25862400
	C	2.51650400	-0.34536500	0.00000000
	C	1.77098000	0.99985300	0.00000000
	C	0.86266100	1.11274800	-1.24837500
	C	0.86266100	1.11274800	1.24837500
	C	0.08431000	2.43601600	-1.21996100
	C	-1.75393800	1.38236500	0.00000000
	C	0.08431000	2.43601600	1.21996100
	H	-0.76015700	-0.00979400	2.15813000
	H	-2.70762400	-1.06498500	0.88344300
	H	-2.70762400	-1.06498500	-0.88344300
	H	-0.76015700	-0.00979400	-2.15813000
	H	3.16819000	-0.40829900	0.88084900
	H	3.16819000	-0.40829900	-0.88084900
	H	2.49709800	1.82526600	0.00000000
	H	1.47641700	1.09246100	-2.15855100
	H	1.47641700	1.09246100	2.15855100
	H	0.77228500	3.29146800	-1.21438500
	H	-0.55877500	2.52404900	-2.10547800
	H	-2.39377000	1.47448300	0.88870700
	H	-2.39377000	1.47448300	-0.88870700
	H	-0.55877500	2.52404900	2.10547800
	H	0.77228500	3.29146800	1.21438500
	N	-0.78800200	2.53529600	0.00000000
	Li	-1.77664900	4.19349700	0.00000000
N-Tri@Na$^+$	C	0.40070800	-1.79973000	1.25605700
	C	1.27862700	-2.02880800	0.00000000
	C	0.40070800	-1.79973000	-1.25605700
	C	-0.81568600	-2.74383300	-1.25697100
	C	-1.67337800	-2.49235500	0.00000000
	C	-0.81568600	-2.74383300	1.25697100
	H	1.00472800	-1.97753600	2.15649400
	H	1.64286300	-3.06421700	0.00000000
	H	1.00472800	-1.97753600	-2.15649400
	H	-1.41346400	-2.58467900	-2.16427700
	H	-0.47887000	-3.78755300	-1.27958500
	H	-2.53922200	-3.16462900	0.00000000
	H	-1.41346400	-2.58467900	2.16427700
	H	-0.47887000	-3.78755300	1.27958500

	C	-0.07516000	-0.32834000	1.25774900
	C	-0.95935500	-0.07109400	0.00000000
	C	-2.16460800	-1.02924100	0.00000000
	C	-0.07516000	-0.32834000	-1.25774900
	C	2.47745100	-1.06541200	0.00000000
	C	1.98452600	0.39139600	0.00000000
	C	1.10960600	0.66392900	-1.24772200
	C	1.10960600	0.66392900	1.24772200
	C	0.57681800	2.10447100	-1.21543200
	C	-1.41250900	1.39860500	0.00000000
	C	0.57681800	2.10447100	1.21543200
	H	-0.68449700	-0.15159800	2.15816400
	H	-2.79082200	-0.84018000	0.88344200
	H	-2.79082200	-0.84018000	-0.88344200
	H	-0.68449700	-0.15159800	-2.15816400
	H	3.10683300	-1.24554300	0.88099200
	H	3.10683300	-1.24554300	-0.88099200
	H	2.84747000	1.07277800	0.00000000
	H	1.70938700	0.53375100	-2.15856100
	H	1.70938700	0.53375100	2.15856100
	H	1.40786900	2.82239700	-1.21233800
	H	-0.03936500	2.30412600	-2.10211300
	H	-2.02655200	1.60354000	0.88805400
	H	-2.02655200	1.60354000	-0.88805400
	H	-0.03936500	2.30412600	2.10211300
	H	1.40786900	2.82239700	1.21233800
	N	-0.26167500	2.35699900	0.00000000
	Na	-1.02271100	4.53882800	0.00000000
N-Tri@K$^+$	C	0.26046700	-2.12758600	1.25653400
	C	1.10745100	-2.44996000	0.00000000
	C	0.26046700	-2.12758600	-1.25653400
	C	-1.05041300	-2.93625800	-1.25640700
	C	-1.87531600	-2.59271400	0.00000000
	C	-1.05041300	-2.93625800	1.25640700
	H	0.84241000	-2.37040600	2.15645000
	H	1.35775900	-3.51878500	0.00000000
	H	0.84241000	-2.37040600	-2.15645000
	H	-1.62840000	-2.71605700	-2.16388800
	H	-0.82666600	-4.01019900	-1.27746800
	H	-2.80852400	-3.16811700	0.00000000
	H	-1.62840000	-2.71605700	2.16388800
	H	-0.82666600	-4.01019900	1.27746800
	C	-0.05341000	-0.61272900	1.25801200
	C	-0.90387000	-0.26151300	0.00000000
	C	-2.20479100	-1.08465800	0.00000000
	C	-0.05341000	-0.61272900	-1.25801200
	C	2.40390200	-1.62171400	0.00000000
	C	2.07063900	-0.12007900	0.00000000
	C	1.23174100	0.24607500	-1.24851400
	C	1.23174100	0.24607500	1.24851400
	C	0.85522900	1.73672200	-1.21099300
	C	-1.19009400	1.25103300	0.00000000
	C	0.85522900	1.73672200	1.21099300
	H	-0.64121300	-0.37125700	2.15790600
	H	-2.80803100	-0.83082900	0.88349500
	H	-2.80803100	-0.83082900	-0.88349500
	H	-0.64121300	-0.37125700	-2.15790600
	H	3.01046200	-1.86816500	0.88114900
	H	3.01046200	-1.86816500	-0.88114900
	H	3.00091300	0.46611000	0.00000000
	H	1.81501900	0.05084500	-2.15869900
	H	1.81501900	0.05084500	2.15869900
	H	1.75910400	2.36079800	-1.20813000
	H	0.26592200	2.00401900	-2.09896900
	H	-1.78097000	1.51861800	0.88836000
	H	-1.78097000	1.51861800	-0.88836000

	H	0.26592200	2.00401900	2.09896900
	H	1.75910400	2.36079800	1.20813000
	N	0.05316700	2.07515400	0.00000000
	K	-0.70044700	4.72436300	0.00000000
N-Tri-Ben@Li$^+$	C	3.10651300	-0.11901100	-1.25838100
	C	3.51624300	-0.92914000	-0.00348900
	C	3.11096100	-0.12184400	1.25463700
	C	3.78154000	1.26528400	1.25515900
	C	3.35304000	2.05162600	0.00012400
	C	3.77709600	1.26811400	-1.25817000
	H	3.40534800	-0.67216600	-2.15957700
	H	4.60484700	-1.06972300	-0.00557200
	H	3.41300000	-0.67701500	2.15351900
	H	3.50438100	1.81659300	2.16354700
	H	4.87265700	1.15265600	1.27389100
	H	3.83071200	3.03841400	0.00038300
	H	3.49672000	1.82144900	-2.16433800
	H	4.86813800	1.15552400	-1.28102200
	C	1.56851800	0.04108100	-1.25714100
	C	1.13402100	0.84822800	0.00270700
	C	1.81995800	2.22737000	0.00304000
	C	1.57297000	0.03822500	1.25922200
	C	2.82348900	-2.30322500	-0.00379800
	C	1.29598800	-2.12361100	-0.00089700
	C	0.84801900	-1.32791900	1.24894400
	C	0.84359700	-1.32507500	-1.24735400
	C	-0.67150000	-1.10683900	1.22018000
	C	-0.39641400	0.98793500	0.00560200
	C	-0.67579900	-1.10409600	-1.21267400
	H	1.26667600	0.60214600	-2.15571300
	H	1.50411700	2.80231300	-0.87916100
	H	1.50725200	2.80034400	0.88763400
	H	1.27432700	0.59727200	2.16011400
	H	3.12817800	-2.88115200	-0.88595200
	H	3.13129700	-2.88312300	0.87597600
	H	0.80827900	-3.10897400	-0.00114400
	H	1.10183800	-1.88942900	2.15816600
	H	1.09415700	-1.88455400	-2.15873000
	H	-1.20334600	-2.06689800	1.21594100
	H	-0.99681500	-0.54694000	2.10639900
	H	-0.72746200	1.54637900	-0.88065300
	H	-0.72420300	1.54436800	0.89434000
	H	-1.00441800	-0.54231900	-2.09648300
	H	-1.20750300	-2.06421200	-1.20853200
	N	-1.09509300	-0.33845700	0.00532600
	C	-4.96317900	0.46112000	1.39557200
	C	-5.19630500	-0.78947700	0.80162600
	C	-5.20890100	-0.91075800	-0.59691000
	C	-4.98841800	0.21846100	-1.40148600
	C	-4.75554000	1.46887200	-0.80749500
	C	-4.74289900	1.59021200	0.59101600
	H	-4.95956400	0.55618100	2.47693100
	H	-5.37310700	-1.66126000	1.42378600
	H	-5.39606800	-1.87625800	-1.05644000
	H	-5.00401400	0.12564400	-2.48291800
	H	-4.59110200	2.34313200	-1.42957100
	H	-4.56861100	2.55823000	1.05027400
	Li	-3.03601900	-0.03354200	0.00914600
N-Tri-Ben@Na$^+$	C	3.47145700	-0.04611900	-1.23461200
	C	3.90085700	-0.81440900	0.03974300
	C	3.42791100	-0.01253300	1.27776000
	C	4.02044000	1.40947500	1.26942800
	C	3.57421400	2.15351400	-0.00521700
	C	4.06385900	1.37599600	-1.24354700
	H	3.81813100	-0.59465200	-2.12143400
	H	4.99550800	-0.89443400	0.05976800

	H	3.74323500	-0.53726000	2.19034700
	H	3.69500300	1.95693400	2.16405600
	H	5.11557700	1.35784100	1.31064300
	H	3.99719500	3.16497300	-0.01131400
	H	3.76975200	1.89942500	-2.16303100
	H	5.15974200	1.32383500	-1.24543700
	C	1.92703600	0.02716300	-1.26393100
	C	1.42570400	0.82836100	-0.02498800
	C	2.03384800	2.24293800	-0.03312600
	C	1.88346600	0.06079500	1.25126900
	C	3.28644600	-2.22505000	0.04768000
	C	1.75133000	-2.13142600	0.01979900
	C	1.23635400	-1.34354000	1.24881300
	C	1.27941000	-1.37674600	-1.24657400
	C	-0.29313000	-1.20512200	1.18565300
	C	-0.11101100	0.87941300	-0.05235300
	C	-0.25128900	-1.23726000	-1.24036700
	H	1.61147400	0.55726500	-2.17656200
	H	1.70328100	2.78677600	-0.92960000
	H	1.67276000	2.81001000	0.83681400
	H	1.53658800	0.61472400	2.13804800
	H	3.64004800	-2.79705000	-0.82001700
	H	3.60958700	-2.77400400	0.94174600
	H	1.31891400	-3.14238400	0.02572300
	H	1.50392900	-1.87639500	2.17138700
	H	1.57862200	-1.93362200	-2.14494800
	H	-0.77114300	-2.19349700	1.18711800
	H	-0.66343300	-0.65191500	2.05904800
	H	-0.45332400	1.40776500	-0.95338600
	H	-0.48386500	1.43133800	0.82210200
	H	-0.59083900	-0.70719300	-2.14011000
	H	-0.72986700	-2.22530500	-1.23267400
	N	-0.73286400	-0.47961000	-0.04506700
	C	-5.24106100	1.12231900	1.18334800
	C	-5.55340900	-0.24124500	1.29232100
	C	-5.77903700	-1.00370400	0.13621400
	C	-5.69170900	-0.40285800	-1.12882900
	C	-5.37934700	0.96075700	-1.23755700
	C	-5.15358800	1.72310000	-0.08148500
	H	-5.09099800	1.71812500	2.07879700
	H	-5.64616500	-0.70044900	2.27202300
	H	-6.04644700	-2.05278300	0.22142200
	H	-5.89169400	-0.98691400	-2.02225500
	H	-5.33644700	1.43166500	-2.21518300
	H	-4.93634100	2.78385400	-0.16469400
	Na	-3.06102300	-0.20748300	-0.07087100
N-Tri-Ben@K$^+$	C	-3.83489000	0.01090600	1.25545500
	C	-4.29862600	-0.76579900	-0.00180100
	C	-3.83285700	0.01243800	-1.25738600
	C	-4.40134500	1.44434100	-1.25733500
	C	-3.92157300	2.19676900	0.00020700
	C	-4.40334300	1.44284500	1.25611400
	H	-4.17608600	-0.52069000	2.15470500
	H	-5.39477300	-0.82717500	-0.00271900
	H	-4.17252700	-0.51814700	-2.15781100
	H	-4.08132500	1.97503000	-2.16402300
	H	-5.49780800	1.41109300	-1.27994700
	H	-4.32758200	3.21528900	0.00046100
	H	-4.08476000	1.97249400	2.16391000
	H	-5.49984000	1.40956800	1.27694900
	C	-2.28930700	0.05754300	1.25806300
	C	-1.79528900	0.83520200	0.00120100
	C	-2.37972800	2.25957100	0.00148900
	C	-2.28727800	0.05913000	-1.25742900
	C	-3.70849600	-2.18687500	-0.00218900
	C	-2.17189000	-2.11928600	-0.00095500

	C	-1.66410300	-1.35608000	-1.24867400
	C	-1.66609900	-1.35768200	1.24850400
	C	-0.13087400	-1.24134200	-1.20854600
	C	-0.25671500	0.85436400	0.00259400
	C	-0.13280000	-1.24313000	1.21091100
	H	-1.94956600	0.59360200	2.15863700
	H	-2.02500300	2.80883500	0.88551200
	H	-2.02356100	2.80972700	-0.88141000
	H	-1.94610500	0.59632500	-2.15679300
	H	-4.05763700	-2.74176000	0.87844600
	H	-4.05634200	-2.74075200	-0.88396800
	H	-1.75661000	-3.13751900	-0.00124500
	H	-1.95776500	-1.89537300	-2.15971800
	H	-1.96124600	-1.89808600	2.15841100
	H	0.33052700	-2.23796600	-1.20659800
	H	0.23437600	-0.70576900	-2.09565400
	H	0.10817300	1.38954800	0.89169600
	H	0.10971800	1.39090500	-0.88509600
	H	0.23128100	-0.70892900	2.09929300
	H	0.32847900	-2.23978900	1.20820700
	N	0.33742500	-0.51088800	0.00208900
	C	6.06412700	0.40152500	-1.39908900
	C	6.25576400	-0.83595700	-0.76908600
	C	6.26646500	-0.91564200	0.63046600
	C	6.08502900	0.24208800	1.39979800
	C	5.89351800	1.47963400	0.76978500
	C	5.88308600	1.55935400	-0.62970900
	H	6.08895700	0.46857500	-2.48296500
	H	6.42917900	-1.72744200	-1.36492700
	H	6.44827700	-1.86881100	1.11860100
	H	6.12672600	0.18557300	2.48376200
	H	5.78725300	2.38150500	1.36577900
	H	5.76824700	2.52291500	-1.11781600
	K	3.10414300	-0.14684600	-0.00171700
N-Tetra@Li$^+$	C	0.67580900	-1.27402200	-0.46868300
	C	2.15266100	-1.22407500	-0.88941900
	C	2.15266100	1.22407500	-0.88941900
	C	0.67580900	1.27402200	-0.46868300
	C	-0.03673400	0.00000000	-0.99992800
	H	2.23377500	-1.22243700	-1.98527700
	H	2.68701600	-2.10686000	-0.51170500
	H	2.68701600	2.10686000	-0.51170500
	H	2.23377500	1.22243700	-1.98527700
	H	0.02142000	0.00000000	-2.10148700
	C	-1.53573000	0.00000000	-0.59021600
	C	-0.02164100	2.52970600	-1.02378300
	C	-1.50320800	2.53580000	-0.59121800
	C	-2.20460900	1.27621500	-1.13692900
	C	-2.20460900	-1.27621500	-1.13692900
	C	-1.50320800	-2.53580000	-0.59121800
	C	-0.02164100	-2.52970600	-1.02378300
	C	0.58479600	-1.25736800	1.08419300
	C	0.58479600	1.25736800	1.08419300
	C	2.76906400	0.00000000	1.13121700
	C	-1.58771600	-2.53872100	0.94800800
	C	-1.58556000	0.00000000	0.96649800
	C	-1.58771600	2.53872100	0.94800800
	C	1.31008900	0.00000000	1.60997500
	C	-0.90157100	1.27763100	1.50510700
	C	-0.90157100	-1.27763100	1.50510700
	H	0.48333600	3.43386500	-0.65572700
	H	0.05223200	2.54451200	-2.12041300
	H	-1.99149100	3.43193300	-0.99125200
	H	-3.26516700	1.28490400	-0.85373500
	H	-2.17216900	1.26797300	-2.23541900
	H	-3.26516700	-1.28490400	-0.85373500

	H	-2.17216900	-1.26797300	-2.23541900
	H	-1.99149100	-3.43193300	-0.99125200
	H	0.48333600	-3.43386500	-0.65572700
	H	0.05223200	-2.54451200	-2.12041300
	H	1.08311300	-2.15624900	1.47918800
	H	1.08311300	2.15624900	1.47918800
	H	3.29797200	-0.88822300	1.50106500
	H	3.29797200	0.88822300	1.50106500
	H	-2.63694000	-2.56456700	1.26682100
	H	-1.11002500	-3.43953600	1.35497700
	H	-2.63821700	0.00000000	1.28260700
	H	-2.63694000	2.56456700	1.26682100
	H	-1.11002500	3.43953600	1.35497700
	H	1.30626500	0.00000000	2.70818000
	H	-0.95919300	1.28049500	2.60238300
	H	-0.95919300	-1.28049500	2.60238300
	N	2.85271000	0.00000000	-0.36864100
	Li	4.69187200	0.00000000	-0.94774000
N-Tetra@Na$^+$	C	0.37475900	0.46938900	1.27377900
	C	0.65980800	1.97885300	1.21898700
	C	0.65980800	1.97885300	-1.21898700
	C	0.37475900	0.46938900	-1.27377900
	C	0.96708500	-0.19372100	0.00000000
	H	1.74475900	2.15512800	1.21664100
	H	0.23959000	2.47667000	2.10411300
	H	0.23959000	2.47667000	-2.10411300
	H	1.74475900	2.15512800	-1.21664100
	H	2.05897000	-0.03621100	0.00000000
	C	0.69473500	-1.72273800	0.00000000
	C	0.98994500	-0.17623100	-2.52878900
	C	0.69196700	-1.69027700	-2.53592400
	C	1.29797700	-2.34074600	-1.27637500
	C	1.29797700	-2.34074600	1.27637500
	C	0.69196700	-1.69027700	2.53592400
	C	0.98994500	-0.17623100	2.52878900
	C	-1.16417400	0.23918400	1.25686600
	C	-1.16417400	0.23918400	-1.25686600
	C	-1.40256700	2.40997000	0.00000000
	C	-0.83387400	-1.91208800	2.53827200
	C	-0.85202000	-1.91148400	0.00000000
	C	-0.83387400	-1.91208800	-2.53827200
	C	-1.75211100	0.91504900	0.00000000
	C	-1.44991200	-1.27837700	-1.27740400
	C	-1.44991200	-1.27837700	1.27740400
	H	0.57953400	0.29424000	-3.43343600
	H	2.07579100	-0.00533800	-2.54291700
	H	1.13341100	-2.14130400	-3.43230600
	H	1.10977200	-3.42233100	-1.28512300
	H	2.38927800	-2.21095200	-1.26848000
	H	1.10977200	-3.42233100	1.28512300
	H	2.38927800	-2.21095200	1.26848000
	H	1.13341100	-2.14130400	3.43230600
	H	0.57953400	0.29424000	3.43343600
	H	2.07579100	-0.00533800	2.54291700
	H	-1.60259700	0.70024400	2.15561400
	H	-1.60259700	0.70024400	-2.15561400
	H	-1.81923600	2.90374000	0.88778200
	H	-1.81923600	2.90374000	-0.88778200
	H	-1.05818800	-2.98561600	2.56431000
	H	-1.28266400	-1.47292100	3.43901500
	H	-1.07371300	-2.98809700	0.00000000
	H	-1.05818800	-2.98561600	-2.56431000
	H	-1.28266400	-1.47292100	-3.43901500
	H	-2.84579000	0.81133900	0.00000000
	H	-2.53767600	-1.43430300	-1.27998000
	H	-2.53767600	-1.43430300	1.27998000

	N	0.07949100	2.62754800	0.00000000
	Na	0.60289700	4.87697100	0.00000000
N-Tetra@K$^+$	C	0.33220500	0.22041700	1.27388000
	C	0.54775700	1.74298800	1.21399700
	C	0.54775700	1.74298800	-1.21399700
	C	0.33220500	0.22041700	-1.27388000
	C	0.95236500	-0.41686100	0.00000000
	H	1.62414100	1.96857600	1.21321400
	H	0.10691200	2.22136200	2.10073400
	H	0.10691200	2.22136200	-2.10073400
	H	1.62414100	1.96857600	-1.21321400
	H	2.03643500	-0.21191900	0.00000000
	C	0.74654600	-1.95679100	0.00000000
	C	0.97403700	-0.39858000	-2.52855600
	C	0.74282900	-1.92464400	-2.53588300
	C	1.37661200	-2.54778500	-1.27616400
	C	1.37661200	-2.54778500	1.27616400
	C	0.74282900	-1.92464400	2.53588300
	C	0.97403700	-0.39858000	2.52855600
	C	-1.19434600	-0.07633300	1.25638100
	C	-1.19434600	-0.07633300	-1.25638100
	C	-1.52415600	2.08121800	0.00000000
	C	-0.77149200	-2.21296300	2.53756300
	C	-0.79013100	-2.21219200	0.00000000
	C	-0.77149200	-2.21296300	-2.53756300
	C	-1.81280700	0.57256100	0.00000000
	C	-1.41468400	-1.60541700	-1.27747700
	C	-1.41468400	-1.60541700	1.27747700
	H	0.54245300	0.05343500	-3.43293800
	H	2.05131500	-0.17959800	-2.54364900
	H	1.20364800	-2.35653400	-3.43214900
	H	1.23617300	-3.63680500	-1.28524600
	H	2.46116400	-2.37005600	-1.26781900
	H	1.23617300	-3.63680500	1.28524600
	H	2.46116400	-2.37005600	1.26781900
	H	1.20364800	-2.35653400	3.43214900
	H	0.54245300	0.05343500	3.43293800
	H	2.05131500	-0.17959800	2.54364900
	H	-1.65236800	0.36534000	2.15529400
	H	-1.65236800	0.36534000	-2.15529400
	H	-1.96466900	2.55581000	0.88766100
	H	-1.96466900	2.55581000	-0.88766100
	H	-0.94783900	-3.29556900	2.56241000
	H	-1.23894300	-1.79513700	3.43906600
	H	-0.96432600	-3.29763900	0.00000000
	H	-0.94783900	-3.29556900	-2.56241000
	H	-1.23894300	-1.79513700	-3.43906600
	H	-2.90065800	0.41800400	0.00000000
	H	-2.49465300	-1.80902300	-1.28000300
	H	-2.49465300	-1.80902300	1.28000300
	N	-0.05910000	2.36118200	0.00000000
	K	0.41271800	5.07051900	0.00000000
N-Tetra-Ben@Li$^+$	C	0.67824300	1.28619100	-0.33089700
	C	-0.84599400	1.25692200	-0.53196000
	C	-0.88527800	-1.18223300	-0.52520300
	C	0.63680300	-1.26031000	-0.32304100
	C	1.28765500	0.00085300	-0.95463200
	H	-1.08885100	1.25363700	-1.60287200
	H	-1.30739300	2.14916300	-0.08756000
	H	-1.37484800	-2.05739400	-0.07629300
	H	-1.12694500	-1.17671200	-1.59642900
	H	1.07066300	0.00105400	-2.03607000
	C	2.82974800	-0.02362000	-0.76530600
	C	1.22764000	-2.52719600	-0.96834000
	C	2.75593400	-2.55847100	-0.75355100
	C	3.39264900	-1.31101200	-1.39805800

	C	3.43452400	1.24089400	-1.40594000
	C	2.83889300	2.51231700	-0.76942000
	C	1.31034400	2.52918000	-0.98391600
	C	0.99239200	1.26914500	1.19178500
	C	0.95102200	-1.24399800	1.19967100
	C	-1.17918300	0.04852600	1.55760600
	C	3.14428000	2.51412500	0.74145600
	C	3.10237600	-0.02333100	0.76824000
	C	3.06104800	-2.56093200	0.75735800
	C	0.33177700	0.02496000	1.82175800
	C	2.48179400	-1.28911300	1.40332600
	C	2.52388400	1.26586400	1.39530900
	H	0.76575200	-3.42282600	-0.52927400
	H	0.99673800	-2.54144200	-2.04295400
	H	3.16754500	-3.46294900	-1.21669400
	H	4.48280400	-1.33749300	-1.26939800
	H	3.20338500	-1.30286200	-2.48058700
	H	4.52494200	1.23250700	-1.27688900
	H	3.24537500	1.23206400	-2.48847900
	H	3.27941900	3.40017800	-1.23805800
	H	0.87788700	3.44207800	-0.55057700
	H	1.07970000	2.54436000	-2.05858600
	H	0.57039600	2.17615300	1.65201000
	H	0.49951300	-2.13393000	1.66533900
	H	-1.63550500	0.94477300	1.99785400
	H	-1.66348100	-0.83015100	2.00376100
	H	4.22900900	2.52193900	0.90565700
	H	2.74638400	3.42359400	1.21077400
	H	4.18948400	-0.04074000	0.93029200
	H	4.14490900	-2.60320800	0.92186900
	H	2.63352200	-3.45400500	1.23212600
	H	0.49862200	0.02556500	2.90760200
	H	2.69698600	-1.29194700	2.48104600
	H	2.73905300	1.26840800	2.47301300
	N	-1.47993400	0.04898000	0.08883100
	Li	-3.43499300	0.04411400	-0.09593900
	C	-5.44282000	1.39630000	-0.10515900
	C	-5.37807700	0.74807000	-1.34852600
	C	-5.34330000	-0.65407500	-1.40818000
	C	-5.37366900	-1.40795800	-0.22439000
	C	-5.43945200	-0.75982200	1.01898200
	C	-5.47476600	0.64222400	1.07857900
	H	-5.47880800	2.48030000	-0.05894400
	H	-5.35955200	1.33097700	-2.26418000
	H	-5.29903000	-1.15536100	-2.37006000
	H	-5.35239500	-2.49233100	-0.27084900
	H	-5.46940700	-1.34293300	1.93420400
	H	-5.53214200	1.14331000	2.03990200
N-Tetra-Ben@Na$^+$	C	0.95375200	1.25781400	-0.33615700
	C	-0.56699900	1.17013400	-0.55072200
	C	-0.51635600	-1.26283100	-0.56011300
	C	1.00716000	-1.28846500	-0.34600700
	C	1.61662100	0.00028200	-0.96250600
	H	-0.79694200	1.16678700	-1.62514700
	H	-1.06275700	2.04417100	-0.10531700
	H	-0.97602000	-2.15946500	-0.12145500
	H	-0.74675500	-1.26086000	-1.63435900
	H	1.40982400	0.00009000	-2.04605300
	C	3.15664800	0.03164400	-0.75882800
	C	1.65151600	-2.52772500	-0.99366300
	C	3.17782800	-2.50424000	-0.76462500
	C	3.77358100	-1.22952200	-1.39446100
	C	3.71974400	1.32213100	-1.38499800
	C	3.07109800	2.56605500	-0.74552500
	C	1.54512300	2.52765500	-0.97471500
	C	1.25371800	1.24131600	1.18955500

	C	1.30684000	-1.27108300	1.17981300
	C	-0.87482900	-0.06145100	1.52203300
	C	3.36173500	2.56855100	0.76829900
	C	3.41476400	0.03133700	0.77735700
	C	3.46879200	-2.50571000	0.74919300
	C	0.63364200	-0.03085000	1.80434600
	C	2.83621700	-1.26096500	1.39799700
	C	2.78218900	1.29354200	1.40772600
	H	1.21913100	-3.44304700	-0.56519600
	H	1.43131000	-2.54333100	-2.07058800
	H	3.62725200	-3.38967900	-1.22955900
	H	4.86273400	-1.21615800	-1.25506300
	H	3.59451500	-1.22087800	-2.47875800
	H	4.80857200	1.35347300	-1.24613000
	H	3.54053400	1.31415800	-2.46928600
	H	3.48318900	3.47288000	-1.20381800
	H	1.07494700	3.42098600	-0.53961200
	H	1.32440400	2.54168800	-2.05154200
	H	0.79354100	2.12882900	1.65156000
	H	0.88469600	-2.18059200	1.63518900
	H	-1.36702700	0.81435400	1.96605000
	H	-1.33006200	-0.96053200	1.95854900
	H	4.44381500	2.61599700	0.94327100
	H	2.92521900	3.45915300	1.23959900
	H	4.50028900	0.05360800	0.94974300
	H	4.55197300	-2.50873800	0.92386500
	H	3.07044300	-3.41733600	1.21401200
	H	0.79035400	-0.03166400	2.89190000
	H	3.04116400	-1.26324500	2.47774400
	H	2.98736100	1.29644300	2.48744200
	N	-1.16027400	-0.06148600	0.05453700
	Na	-3.48570700	-0.07641700	-0.22668500
	C	-5.98590400	0.80906800	-1.24757900
	C	-6.03886000	-0.58918200	-1.35108400
	C	-6.00772400	-1.37999400	-0.19212000
	C	-5.92405400	-0.77222000	1.06946300
	C	-5.87115300	0.62602400	1.17293200
	C	-5.90185200	1.41671400	0.01447100
	H	-6.03560500	1.42195400	-2.14271200
	H	-6.12977700	-1.05843800	-2.32620200
	H	-6.07470500	-2.46104800	-0.27071800
	H	-5.92508200	-1.38263800	1.96766900
	H	-5.82959700	1.09634200	2.15085500
	H	-5.88566200	2.49954500	0.09537200
N-Tetra-Ben@K$^+$	C	1.27568700	1.24322100	-0.33797500
	C	-0.24232900	1.11667300	-0.55957500
	C	-0.13673000	-1.30667100	-0.57411500
	C	1.38730500	-1.30174200	-0.35444300
	C	1.97046400	0.00262300	-0.96394200
	H	-0.46578800	1.11149800	-1.63581000
	H	-0.76043100	1.97973200	-0.11619600
	H	-0.57796300	-2.21546300	-0.14030100
	H	-0.36223500	-1.30888600	-1.64977200
	H	1.76931600	0.00074900	-2.04865800
	C	3.50825700	0.06861300	-0.75248600
	C	2.06409800	-2.52349300	-1.00152300
	C	3.58829600	-2.46599400	-0.76519800
	C	4.15764600	-1.17612900	-1.38835000
	C	4.04520200	1.37329900	-1.37219100
	C	3.36529100	2.60034000	-0.73261900
	C	1.84182200	2.52751200	-0.96958400
	C	1.56872200	1.22874000	1.18943900
	C	1.67970000	-1.28121000	1.17314200
	C	-0.53099100	-0.12268200	1.50236800
	C	3.64814900	2.60497900	0.78276100
	C	3.75903200	0.06993400	0.78497200

	C	3.87185400	-2.46472900	0.75018300
	C	0.97482100	-0.05872500	1.79828200
	C	3.20724600	-1.23689800	1.39923300
	C	3.09434900	1.31540300	1.41561800
	H	1.65079800	-3.44977500	-0.57755600
	H	1.84930100	-2.54153100	-2.07960400
	H	4.06080800	-3.33956300	-1.22996900
	H	5.24564000	-1.13804800	-1.24352600
	H	3.98359700	-1.16837300	-2.47351300
	H	5.13251700	1.42885500	-1.22821200
	H	3.87109600	1.36439500	-2.45735500
	H	3.75954400	3.51755800	-1.18620300
	H	1.34914300	3.40875500	-0.53443600
	H	1.62638300	2.53974800	-2.04758500
	H	1.08614400	2.10444100	1.65157500
	H	1.27664500	-2.20167000	1.62413500
	H	-1.04396700	0.74136000	1.94832400
	H	-0.96774900	-1.03312600	1.93612800
	H	4.72802100	2.67688000	0.96362600
	H	3.18866000	3.48405600	1.25405300
	H	4.84302600	0.11673500	0.96284500
	H	4.95403900	-2.44335200	0.93042900
	H	3.49221400	-3.38665500	1.21049300
	H	1.12656600	-0.05899800	2.88672500
	H	3.40705300	-1.23746600	2.48002100
	H	3.29427000	1.31987300	2.49641400
	N	-0.80625200	-0.12521900	0.03859900
	C	-6.61372500	0.54568100	-1.35868400
	C	-6.69198700	-0.83418900	-1.12395600
	C	-6.65530300	-1.32567900	0.18843600
	C	-6.54044100	-0.43719400	1.26664000
	C	-6.46192300	0.94252200	1.03186400
	C	-6.49862800	1.43405600	-0.28043400
	H	-6.67526100	0.92815000	-2.37346000
	H	-6.81432800	-1.52052000	-1.95698600
	H	-6.74929500	-2.39219500	0.37173800
	H	-6.54475100	-0.81519700	2.28492900
	H	-6.40616000	1.63324500	1.86835700
	H	-6.47083400	2.50495500	-0.46001500
	K	-3.58039800	-0.15595900	-0.22042100
N-Penta @Li^{+}	C	1.91024100	-0.64402300	1.43559000
	C	2.59894600	-1.84704100	0.78903900
	C	0.51291800	-2.47349300	-0.30074800
	C	-0.25700600	-1.27371300	0.29712900
	C	0.41340000	-0.93373400	1.66184200
	C	2.10211500	-0.96925300	-1.43822900
	C	-0.13550700	-0.04089300	-0.67187200
	C	2.03508500	0.58556000	0.51780000
	C	1.39005000	0.27377500	-0.87244400
	C	1.36121100	1.81848400	1.14848600
	C	-0.82198500	1.20657400	-0.00139500
	C	-0.28797100	0.27552200	2.30769700
	C	-0.13113400	1.48764200	1.36822400
	C	-1.76430600	-1.58888900	0.51808900
	C	-2.32371800	0.86397000	0.23182200
	C	-1.76945800	-0.04224300	2.53867100
	C	-2.42910900	-0.35431900	1.19015800
	C	1.53933200	3.03799000	0.23213200
	C	0.88069700	2.73815400	-1.12488400
	C	-0.61968100	2.45784700	-0.89383700
	C	1.57217400	1.51388400	-1.77266900
	C	-0.88428200	-0.36715300	-2.00057400
	C	-2.48895800	-1.89802900	-0.80605600
	C	-2.37353500	-0.68233700	-1.74300700
	C	-3.05040100	0.53287300	-1.08469200
	H	2.39706100	-0.43828200	2.39850100

	H	2.51960600	-2.73536500	1.42971700
	H	3.66466900	-1.64293000	0.62192000
	H	0.08633300	-2.79586400	-1.25445300
	H	0.45781700	-3.32562200	0.39065500
	H	0.30695600	-1.80585600	2.32633100
	H	3.17412700	-0.76231900	-1.55740600
	H	1.70649900	-1.23846700	-2.42476900
	H	3.10141200	0.80705800	0.35373100
	H	1.82986000	2.01733100	2.12250100
	H	0.20011000	0.49825600	3.26682800
	H	-0.62477300	2.35671100	1.82612400
	H	-1.84910300	-2.45051000	1.19751400
	H	-2.80485200	1.72972900	0.70829800
	H	-1.87515900	-0.89447500	3.22321100
	H	-2.26889300	0.81092600	3.01468100
	H	-3.49117200	-0.58249400	1.34879600
	H	1.07973900	3.92365600	0.68773200
	H	2.60655000	3.26297500	0.10481000
	H	0.99019300	3.60155400	-1.79155800
	H	-1.07946600	3.32255200	-0.39730400
	H	-1.12840100	2.35664100	-1.85559700
	H	2.64381100	1.72300400	-1.89820700
	H	1.17239800	1.33314200	-2.77720400
	H	-0.81061600	0.46932800	-2.69909100
	H	-0.42879700	-1.21814600	-2.51936300
	H	-2.08383300	-2.79773400	-1.28736100
	H	-3.54380300	-2.11617900	-0.59895100
	H	-2.86084300	-0.90569300	-2.69996600
	H	-3.05106100	1.38938500	-1.76735800
	H	-4.10333300	0.30681400	-0.87460800
	N	1.96859500	-2.16744200	-0.53276900
	Li	2.80403300	-3.69665600	-1.34880400
N-Penta @Na^{+}	C	1.44324300	0.89212100	1.66887400
	C	2.82239700	0.38206600	1.24347800
	C	1.80024700	-1.51088800	0.12066200
	C	0.36536800	-1.06376300	0.48715600
	C	0.45900700	-0.28343000	1.83157600
	C	2.21090300	0.57718400	-1.10611500
	C	-0.18822500	-0.11539200	-0.63709800
	C	0.88736000	1.84471000	0.59540800
	C	0.79874000	1.09964900	-0.77586100
	C	-0.49797500	2.38634600	0.99649900
	C	-1.59757500	0.43192500	-0.19966100
	C	-0.93415900	0.22224400	2.25025600
	C	-1.45119900	1.18129200	1.15975200
	C	-0.61025800	-2.26581100	0.64815700
	C	-2.55260500	-0.78714900	-0.02235000
	C	-1.88893300	-0.96480500	2.42245200
	C	-1.99586200	-1.71626400	1.09054400
	C	-1.00461400	3.36648000	-0.07153900
	C	-1.11781500	2.62275500	-1.41291300
	C	-2.11200500	1.45371200	-1.24509800
	C	0.27768600	2.09789200	-1.83011600
	C	-0.35802900	-0.93451900	-1.95376300
	C	-0.77296000	-3.05709400	-0.66320500
	C	-1.32375400	-2.12277000	-1.75488700
	C	-2.70359200	-1.59451400	-1.32458100
	H	1.54326900	1.42720700	2.62335700
	H	3.23632700	-0.29896700	1.99922400
	H	3.52272400	1.21933700	1.12181900
	H	1.81935400	-2.09760100	-0.80170300
	H	2.19909600	-2.14793400	0.92229400
	H	0.83692200	-0.97204700	2.60396100
	H	2.90824300	1.42272800	-1.18372500
	H	2.22306900	0.05235600	-2.06884200
	H	1.57915300	2.69321100	0.47357400

	H	-0.40882300	2.90442800	1.96174100
	H	-0.84342000	0.77043900	3.19851000
	H	-2.44477200	1.54930100	1.45372000
	H	-0.22502300	-2.92999400	1.43668900
	H	-3.53685400	-0.41164900	0.29179700
	H	-1.52534300	-1.63603000	3.21208700
	H	-2.87912500	-0.61175400	2.73717100
	H	-2.67930700	-2.56778000	1.20693800
	H	-1.98143300	3.77243400	0.21902400
	H	-0.31769100	4.21883100	-0.15807400
	H	-1.48718300	3.30546200	-2.18732800
	H	-3.08100100	1.84559000	-0.90791900
	H	-2.29811400	0.98279100	-2.21351900
	H	0.97580300	2.94295000	-1.91256400
	H	0.23347400	1.63436000	-2.82269000
	H	-0.73416600	-0.29690500	-2.75695400
	H	0.60303800	-1.31698900	-2.31429700
	H	0.17554600	-3.50796800	-0.98246600
	H	-1.46471900	-3.89252900	-0.49876700
	H	-1.41454200	-2.67129800	-2.70057500
	H	-3.14793500	-0.98727500	-2.12064200
	H	-3.39015100	-2.43403400	-1.15673000
	N	2.74019300	-0.35420900	-0.05353300
	Na	4.82635400	-1.12118800	-0.67328400
N-Penta @K^+	C	0.95381900	1.16769200	1.74665200
	C	2.41745500	0.85746100	1.41910000
	C	1.76602500	-1.18546500	0.30148900
	C	0.25820700	-0.95860600	0.56685900
	C	0.14773000	-0.13865900	1.88744000
	C	1.93952600	0.90464000	-0.95933600
	C	-0.35597000	-0.12858700	-0.61882100
	C	0.33267700	1.99978300	0.61012700
	C	0.44497300	1.21696200	-0.73860600
	C	-1.14120200	2.33341800	0.90859400
	C	-1.85695500	0.20609800	-0.28649800
	C	-1.33002700	0.15785600	2.20368900
	C	-1.91215700	1.00274100	1.05307800
	C	-0.53474000	-2.28893000	0.70668100
	C	-2.62803400	-1.13814800	-0.12880500
	C	-2.10537400	-1.15551100	2.35616000
	C	-2.01310700	-1.94751100	1.04607800
	C	-1.72137200	3.19936400	-0.21927100
	C	-1.63421800	2.41603400	-1.54006300
	C	-2.44956200	1.11314400	-1.39424600
	C	-0.15133300	2.10053400	-1.85392200
	C	-0.31365800	-0.99340500	-1.91635100
	C	-0.48972800	-3.12532100	-0.58688500
	C	-1.10135200	-2.30943300	-1.74029100
	C	-2.57045800	-1.98869400	-1.41152100
	H	0.90785300	1.73310300	2.68786200
	H	2.87618500	0.26362100	2.22195600
	H	2.99500600	1.78652200	1.31604300
	H	1.93136000	-1.78389900	-0.59885100
	H	2.20226800	-1.73958800	1.14511900
	H	0.57425700	-0.74262200	2.70429200
	H	2.50572800	1.84467500	-1.02130800
	H	2.09269000	0.36806100	-1.90349900
	H	0.89596100	2.94050200	0.50280700
	H	-1.19482300	2.88094400	1.86023800
	H	-1.38621800	0.73475300	3.13764000
	H	-2.96651100	1.22413100	1.27349900
	H	-0.10575200	-2.86938000	1.53770800
	H	-3.67614100	-0.90900400	0.11086400
	H	-1.69661300	-1.74501000	3.18788000
	H	-3.15565600	-0.94949600	2.59852500
	H	-2.56854200	-2.88922200	1.14947700

	H	-2.76541600	3.45651900	-0.00089400
	H	-1.16886600	4.14571100	-0.29174800
	H	-2.05250800	3.01592900	-2.35714700
	H	-3.48657400	1.36029100	-1.13007600
	H	-2.49865100	0.59727300	-2.35640300
	H	0.41597200	3.03969300	-1.92043200
	H	-0.06104400	1.61357300	-2.83202400
	H	-0.72717400	-0.43823100	-2.76155400
	H	0.71569900	-1.23461300	-2.20376500
	H	0.53549100	-3.43159200	-0.83289400
	H	-1.05601400	-4.05329000	-0.43921400
	H	-1.04647100	-2.88601900	-2.67214000
	H	-3.04829100	-1.47416000	-2.25206300
	H	-3.13253600	-2.91886300	-1.25960700
	N	2.52729400	0.09027400	0.14908200
	K	5.14459300	-0.49878800	-0.42693900
N-Penta -Ben@ Li^+	C	-0.10863100	-1.17864200	1.76748000
	C	-1.58169800	-0.90597300	1.46414900
	C	-0.99098100	1.15117100	0.31466900
	C	0.52222300	0.95294300	0.56409700
	C	0.66795700	0.14609900	1.88933700
	C	-1.13329100	-0.96278400	-0.93244500
	C	1.14134600	0.12923100	-0.62280700
	C	0.51482400	-2.00534700	0.62851200
	C	0.36846000	-1.23455900	-0.72318400
	C	1.99845700	-2.30548100	0.91084800
	C	2.65273400	-0.17099500	-0.30556600
	C	2.15456000	-0.11755000	2.19026000
	C	2.74140800	-0.95771500	1.03838400
	C	1.28818300	2.30157700	0.68677600
	C	3.39673900	1.18999300	-0.16424400
	C	2.90245100	1.21315000	2.32615000
	C	2.77726600	1.99386100	1.01195000
	C	2.58357200	-3.16578400	-0.21881700
	C	2.46352200	-2.39265600	-1.54310300
	C	3.25188500	-1.07151400	-1.41508500
	C	0.97046900	-2.11222800	-1.84096300
	C	1.06641700	0.98488100	-1.92545800
	C	1.21117900	3.12821300	-0.61158300
	C	1.82861800	2.31803900	-1.76585400
	C	3.30760200	2.03099900	-1.45150200
	H	-0.03832300	-1.73617800	2.71179700
	H	-2.04372000	-0.31365600	2.26512700
	H	-2.13970400	-1.84796000	1.37561000
	H	-1.18542700	1.73255700	-0.58890700
	H	-1.43312000	1.70052000	1.15649600
	H	0.23780600	0.74621200	2.70696500
	H	-1.67936500	-1.91479400	-0.97816900
	H	-1.31514400	-0.43451100	-1.87429000
	H	-0.02986500	-2.95841400	0.53520200
	H	2.07492800	-2.84602600	1.86493200
	H	2.23262300	-0.68718600	3.12709600
	H	3.80287200	-1.15426600	1.24765500
	H	0.85606400	2.87828700	1.51862400
	H	4.45185900	0.98445000	0.06584800
	H	2.49002600	1.79869500	3.15884800
	H	3.95969400	1.03211000	2.55771600
	H	3.31241000	2.94849200	1.10212400
	H	3.63539500	-3.39915800	-0.01142600
	H	2.05072200	-4.12421400	-0.27880000
	H	2.88469800	-2.98849400	-2.36160300
	H	4.29712400	-1.29430100	-1.16201600
	H	3.27792000	-0.56040000	-2.38067300
	H	0.42381400	-3.06424400	-1.89466900
	H	0.85747800	-1.63303600	-2.82027800
	H	1.48244200	0.43271100	-2.77146300

	H	0.02938900	1.20303600	-2.20286700
	H	0.17711500	3.40995100	-0.84885000
	H	1.75836900	4.06934800	-0.47578300
	H	1.75094800	2.88701100	-2.70062600
	H	3.78760600	1.52166100	-2.29399700
	H	3.85097800	2.97399900	-1.31120200
	N	-1.73026900	-0.14899700	0.18289500
	C	-5.56892700	0.13962700	-1.56947700
	C	-5.52428700	1.37575400	-0.90310200
	C	-5.59184100	1.42011100	0.49793100
	C	-5.70147400	0.22918700	1.23272500
	C	-5.74300300	-1.00583400	0.56740700
	C	-5.67756500	-1.05078000	-0.83401400
	H	-5.52423100	0.10372400	-2.65350100
	H	-5.44584200	2.29625300	-1.47298000
	H	-5.56616700	2.37524600	1.01314300
	H	-5.75916300	0.26376100	2.31615600
	H	-5.83571700	-1.92569900	1.13636200
	H	-5.71882000	-2.00548800	-1.34901100
	Li	-3.66160400	0.05700500	-0.09655900
N-Penta-Ben@Na$^+$	C	0.51326700	-1.43907500	1.83745400
	C	-1.01055600	-1.37915600	1.69741300
	C	-0.83093500	0.81005800	0.61104900
	C	0.70816500	0.81912400	0.70137200
	C	1.10228300	-0.01802300	1.95856700
	C	-0.80857100	-1.26299000	-0.74533600
	C	1.30312200	0.14268900	-0.58902200
	C	1.12357400	-2.11424000	0.59442200
	C	0.72937000	-1.31734300	-0.69266400
	C	2.65716000	-2.19995600	0.71237500
	C	2.86721600	0.05702100	-0.43924100
	C	2.63610300	-0.06999200	2.09517300
	C	3.20906400	-0.76461400	0.84228000
	C	1.27976600	2.25703100	0.82483300
	C	3.42020700	1.50221500	-0.29590900
	C	3.19464700	1.34921200	2.23253200
	C	2.82246300	2.15685400	0.98298900
	C	3.23256700	-2.91884600	-0.51875600
	C	2.86331700	-2.11719500	-1.77836300
	C	3.46191300	-0.69815300	-1.65494800
	C	1.32427200	-2.05158800	-1.91246500
	C	0.96968600	1.03509900	-1.82565600
	C	0.94931500	3.11835700	-0.41013500
	C	1.54600200	2.45418100	-1.66703000
	C	3.07670500	2.37150400	-1.51909300
	H	0.75854300	-2.02078100	2.73436200
	H	-1.45940700	-0.90289400	2.57874200
	H	-1.42998500	-2.39025500	1.61074600
	H	-1.18548900	1.41209900	-0.23554100
	H	-1.24773500	1.25902800	1.52487400
	H	0.68405400	0.47791500	2.84885200
	H	-1.21611300	-2.28198700	-0.79855300
	H	-1.15029800	-0.73007000	-1.64226400
	H	0.71734200	-3.13324700	0.49826800
	H	2.90957800	-2.76188400	1.62197800
	H	2.89404000	-0.66136300	2.98486200
	H	4.30321300	-0.81122800	0.93334500
	H	0.86284400	2.72813100	1.72820800
	H	4.51161400	1.44310800	-0.18493300
	H	2.79684700	1.83247700	3.13538400
	H	4.28465000	1.31443700	2.34681100
	H	3.22277200	3.17421100	1.07571200
	H	4.32217000	-3.00230100	-0.43150500
	H	2.83803200	-3.94189500	-0.58083900
	H	3.27458700	-2.60863900	-2.66708300
	H	4.54833300	-0.77270500	-1.52105000

	H	3.30979400	-0.14703300	-2.58819400
	H	0.91509300	-3.07033900	-1.96604400
	H	1.04085800	-1.55675700	-2.84887400
	H	1.36778400	0.58792300	-2.73830800
	H	-0.11167500	1.11172700	-1.98925100
	H	-0.13354000	3.25864300	-0.52367900
	H	1.37199900	4.12085400	-0.27625400
	H	1.29005800	3.04407800	-2.55512100
	H	3.53410600	1.97502400	-2.43297300
	H	3.49144700	3.37642300	-1.37788800
	N	-1.40165200	-0.58561900	0.47256600
	C	-5.62340300	1.36545600	-0.89298300
	C	-5.87640800	1.41215000	0.47823500
	C	-6.31346400	0.25681900	1.14478400
	C	-6.49410600	-0.93280400	0.41966000
	C	-6.24618400	-0.96899800	-0.95977900
	C	-5.81025100	0.18502600	-1.61335200
	H	-5.30077500	2.26519200	-1.40843200
	H	-5.75068200	2.34385800	1.02114300
	H	-6.52415200	0.28443200	2.21119300
	H	-6.85246200	-1.82485900	0.92795800
	H	-6.40651900	-1.88564400	-1.51867600
	H	-5.63044500	0.16967900	-2.68275800
	Na	-3.71788700	-0.34681400	0.19703500
N-Penta -Ben@ K^+	C	0.84406600	-1.47934100	1.78776300
	C	-0.67819000	-1.45454100	1.61547500
	C	-0.55710100	0.72514700	0.58137400
	C	0.98578100	0.79432200	0.69029200
	C	1.39112600	-0.04625900	1.93825400
	C	-0.44976400	-1.29347600	-0.79207800
	C	1.62493900	0.16082000	-0.59914800
	C	1.49547000	-2.11528800	0.54637300
	C	1.09235500	-1.31024300	-0.73182800
	C	3.02921700	-2.16103600	0.68539400
	C	3.18934900	0.11836000	-0.42909800
	C	2.92333600	-0.05538100	2.09703400
	C	3.53754400	-0.71153600	0.84431200
	C	1.51559800	2.24752200	0.84392200
	C	3.69637200	1.58056100	-0.25508800
	C	3.44022200	1.37785600	2.26293700
	C	3.05948600	2.19407600	1.02207900
	C	3.64591500	-2.84164600	-0.54548700
	C	3.27137300	-2.03176700	-1.79825100
	C	3.82909500	-0.60056600	-1.64443700
	C	1.73107200	-2.00476300	-1.95234600
	C	1.28310300	1.05894100	-1.82767200
	C	1.17662500	3.11809900	-0.38123400
	C	1.81228900	2.49578800	-1.63775400
	C	3.34174400	2.46146400	-1.46718200
	H	1.09654100	-2.06797000	2.68095800
	H	-1.16074000	-1.00502100	2.49443300
	H	-1.07030900	-2.47452000	1.50357000
	H	-0.93146200	1.31995700	-0.25697800
	H	-1.00254300	1.14029100	1.49716600
	H	0.94281500	0.42302800	2.82864500
	H	-0.82592100	-2.32340300	-0.86451000
	H	-0.80407400	-0.75686500	-1.68084400
	H	1.11845600	-3.14367800	0.42922300
	H	3.28572300	-2.72974100	1.59047600
	H	3.18705600	-0.65217500	2.98171600
	H	4.63201900	-0.72587500	0.95210400
	H	1.07063600	2.69128300	1.74772600
	H	4.78814700	1.55542600	-0.12794900
	H	3.01414300	1.83531000	3.16617200
	H	4.53010600	1.37522900	2.39269400
	H	3.42802800	3.22242100	1.13644100

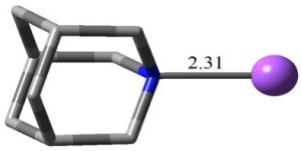
	H	4.73703600	-2.89494500	-0.44266900
	H	3.28203200	-3.87445100	-0.62841700
	H	3.71127900	-2.49816900	-2.68807400
	H	4.91631600	-0.64698800	-1.49472800
	H	3.67584300	-0.04273900	-2.57185300
	H	1.35300500	-3.03424100	-2.02711600
	H	1.44629200	-1.50310100	-2.88519300
	H	1.70999400	0.63836300	-2.74101300
	H	0.20300300	1.09917400	-2.00469900
	H	0.09190300	3.22544600	-0.51013900
	H	1.56580000	4.13210000	-0.22523300
	H	1.55070300	3.09347900	-2.52005300
	H	3.82294700	2.09498500	-2.38034600
	H	3.72336000	3.47756400	-1.30474500
	N	-1.06537000	-0.66749700	0.41620400
	K	-3.83137500	-0.49630300	0.15584400
	C	-6.31362100	1.42159400	-0.92136700
	C	-6.48113600	1.48055600	0.46914800
	C	-6.88277800	0.33851600	1.17572300
	C	-7.11685700	-0.86256100	0.49187700
	C	-6.94895300	-0.92162800	-0.89853200
	C	-6.54737200	0.22051000	-1.60522800
	H	-6.03257200	2.31438300	-1.47255500
	H	-6.32969700	2.41888200	0.99493200
	H	-7.04316400	0.39261600	2.24865900
	H	-7.45881100	-1.73873600	1.03521000
	H	-7.16279500	-1.84304600	-1.43250100
	H	-6.44920400	0.18337300	-2.68635700

Supplementary Table S2: Energies (in kcal mol^{-1}) of the individual system optimized at B3LYP/6-31++G(d,p) level of theory.

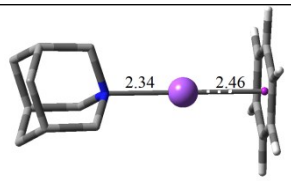
System	Total electronic energy
N-ada	-255254.5907
N-di	-352429.1145
N-tri	-449603.3558
N-tetra	-546778.7982
N-penta	-643941.9016
Li^+	-4571.15511
Na^+	-101707.6026
K^+	-376333.4472
Benzene	-145750.79
N-Ada@Li^+	-259873.23
N-Ada@Na^+	-356995.18
N-Ada@K^+	-631609.67
N-Di@Li^+	-357048.52
N-Di@Na^+	-454170.46
N-Di@K^+	-728784.83
N-Tri@Li^+	-454223.68
N-Tri@Na^+	-551345.57
N-Tri@K^+	-825959.50
N-Tetra@Li^+	-551399.50
N-Tetra@Na^+	-648521.33
N-Tetra@K^+	-923135.44
N-Penta@Li^+	-648563.42
N-Penta@Na^+	-745684.66
N-Penta@K^+	-1020299.28
N-Ada-Ben@Li^+	-405649.7646
N-Ada-Ben@Na^+	-502763.7661
N-Ada-Ben@K^+	-777372.3179
N-Di-Ben@Li^+	-502824.8774
N-Di-Ben@Na^+	-599938.8176
N-Di-Ben@K^+	-874547.2057
N-Tri-Ben@Li^+	-599999.7224
N-Tri-Ben@Na^+	-697113.8491
N-Tri-Ben@K^+	-971722.2791
N-Tetra-Ben@Li^+	-697175.4419
N-Tetra-Ben@Na^+	-794289.479
N-Tetra-Ben@K^+	-1068897.83
N-Penta-Ben@Li^+	-794339.1619
N-Penta-Ben@Na^+	-891452.9359
N-Penta-Ben@K^+	-1166061.287

Supplementary Table S3: BSSE correction energies (in kcal mol^{-1}) obtained at different level of theories

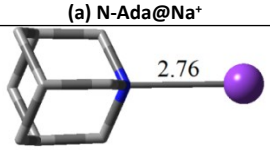
Complexes	B3LYP/		M06-2X		ωB97X-D	
	631++G(d,p)	6-311++G(d,p)	6-31++G(d,p)	6-311++G(d,p)	6-31++G(d,p)	6-311++G(d,p)
N-Ada@Li$^+$	0.47	0.35	0.54	0.48	0.38	0.30
N-Ada@Na$^+$	1.18	0.83	1.06	0.83	1.14	0.69
N-Ada@K$^+$	0.45	0.26	0.28	0.24	0.56	0.27
N-Di@Li$^+$	0.47	0.46	0.51	0.48	0.36	0.37
N-Di@Na$^+$	1.22	0.82	1.10	0.80	1.18	0.66
N-Di@K$^+$	0.49	0.25	0.30	0.28	0.62	0.25
N-Tri@Li$^+$	0.48	0.43	0.55	0.52	0.38	0.33
N-Tri@Na$^+$	1.12	0.83	1.13	0.80	1.20	0.65
N-Tri@K$^+$	0.56	0.25	0.37	0.25	0.65	0.25
N-Tetra@Li$^+$	0.49	0.40	0.56	0.53	0.38	0.33
N-Tetra@Na$^+$	1.27	0.83	1.16	0.80	1.23	0.64
N-Tetra@K$^+$	0.58	0.25	0.41	0.27	0.67	0.25
N-Penta@Li$^+$	0.48	0.40	0.55	0.53	0.35	0.33
N-Penta@Na$^+$	1.24	0.85	1.12	0.80	1.20	0.65
N-Penta@K$^+$	0.61	0.26	0.43	0.27	0.69	0.22
N-Ada-Ben@Li$^+$	1.55	1.52	1.47	1.46	1.18	1.14
N-Ada-Ben@Na$^+$	1.85	1.57	1.64	1.57	1.70	1.33
N-Ada-Ben@K$^+$	0.99	0.64	0.64	0.62	0.99	0.60
N-Di-Ben@Li$^+$	1.58	1.48	1.50	1.40	1.22	1.20
N-Di-Ben@Na$^+$	1.90	0.82	1.67	1.54	1.73	1.27
N-Di-Ben@K$^+$	1.10	0.61	0.72	0.59	1.10	0.56
N-Tri-Ben@Li$^+$	1.56	1.47	1.49	1.30	1.20	1.17
N-Tri-Ben@Na$^+$	1.89	1.55	1.67	1.55	1.73	1.29
N-Tri-Ben@K$^+$	1.13	0.61	0.76	0.62	1.14	0.55
N-Tetra-Ben@Li$^+$	1.57	1.46	1.50	1.47	1.21	1.15
N-Tetra-Ben@Na$^+$	1.90	1.56	1.68	1.56	1.74	1.28
N-Tetra-Ben@K$^+$	1.17	0.62	0.77	0.61	1.19	0.57
N-Penta-Ben@Li$^+$	1.61	1.45	1.52	1.47	1.23	1.20
N-Penta-Ben@Na$^+$	1.94	1.59	1.73	1.31	1.78	1.30
N-Penta-Ben@K$^+$	1.16	0.64	0.77	0.65	1.17	0.57



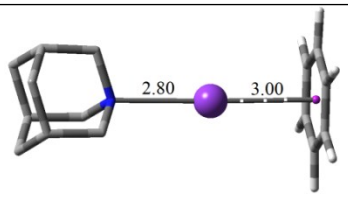
(a) N-Ada@Na^+



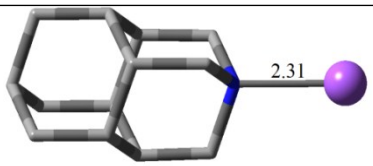
(b) N-Ada-Ben@Na^+



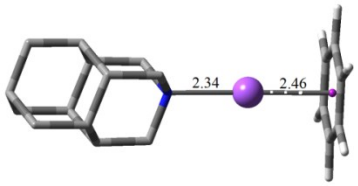
(c) N-Ada@K^+



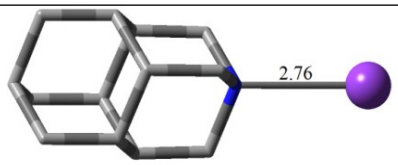
(d) N-Ada-Ben@K^+



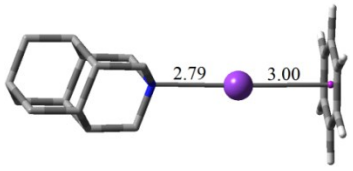
(e) N-Di@Na^+



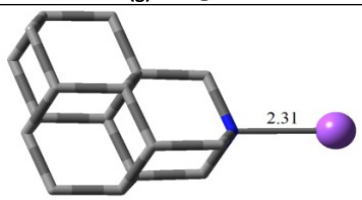
(f) N-Di-Ben@Na^+



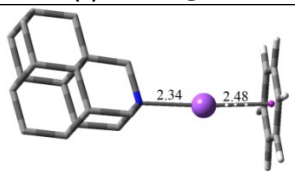
(g) N-Di@K^+



(h) N-Di-Ben@K^+



(i) N-Tri@Na^+



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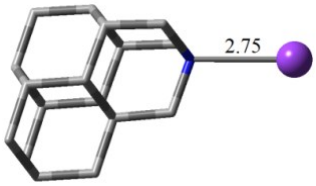

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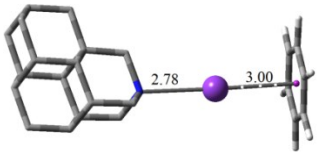

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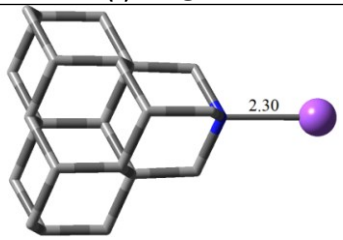
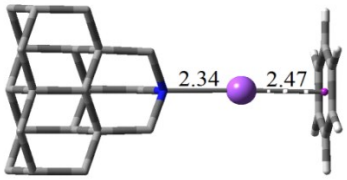


(m) N-Tetra@Na^+



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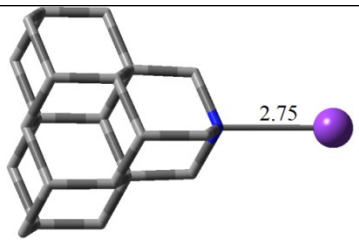
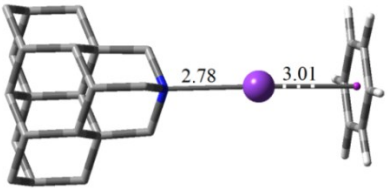
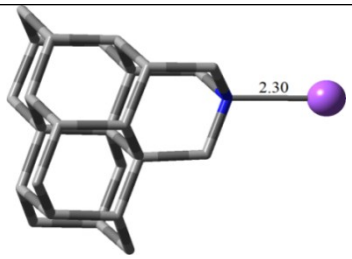


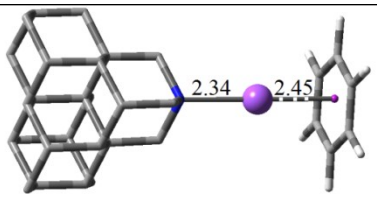
(o) N-Tetra@K^+



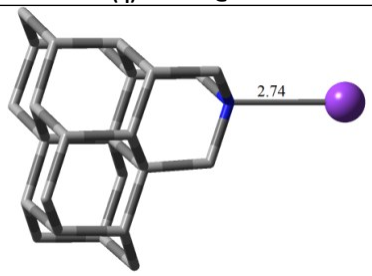
(p) N-Tetra-Ben@K^+



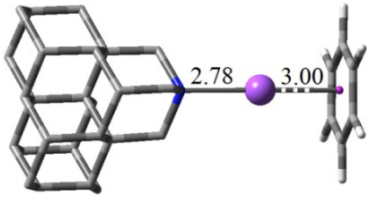
(q) N-Penta@Na^+



(r) N-Penta-Ben@Na^+

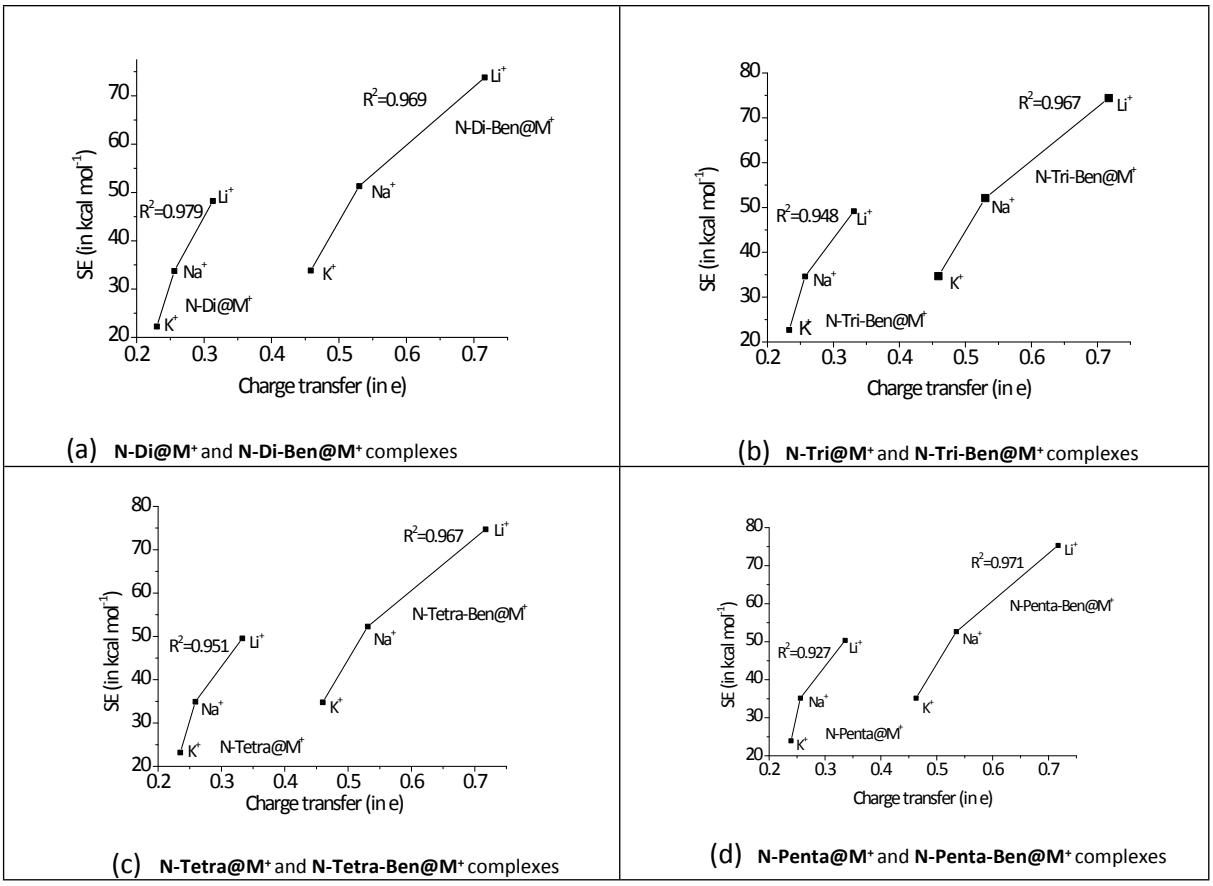


(s) N-Penta@K^+

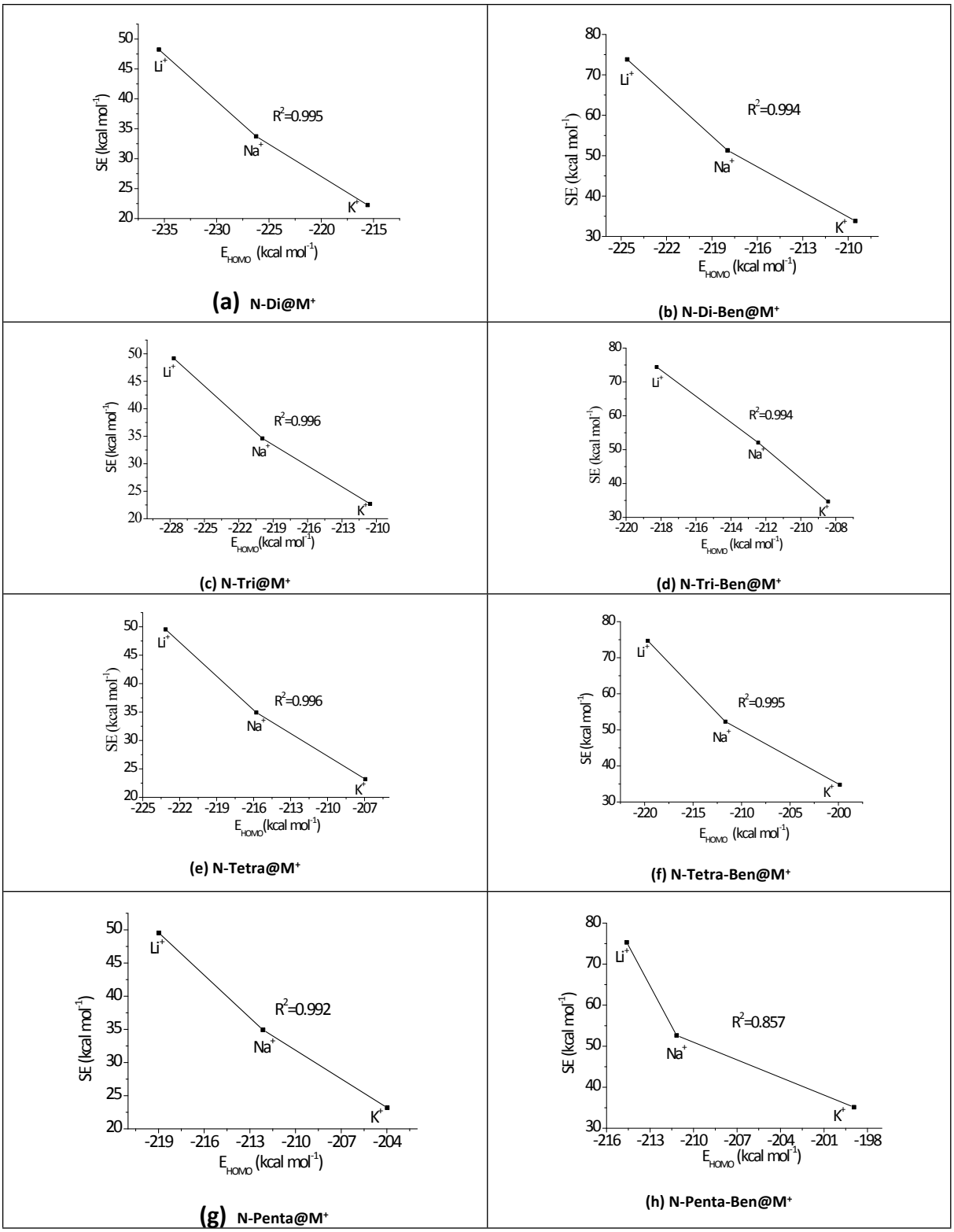


(t) N-Penta-Ben@K^+

Supplementary Fig.S1: Optimised structure of the lone pair-cation and Cation-pi sandwiches complexes. Bond length values are in Å



Supplementary Fig. S2: Plots of SE vs charge transfer for the higher diamondoids (obtained at B3LYP/6-31++G(d,p) level of theory).



Supplementary Fig. S3: Plots of SE and E_{HOMO} for the cation-lone pairs and sandwiches obtained at B3LYP/6-31++G(d,p) level of theory.