

Ng@M₁₀H₁₀: Nobel Gas Trapping By Alkali Hydride Cage

Farnaz Yashmin, Kangkan Sarmah, Pankaz K. Sharma*, Ankur K. Guha*

Department of Chemistry, Cotton University,

Panbazar, Guwahati, Assam, INDIA-781001

*Email: pankaz.sharma@gmail.com

Supporting Information

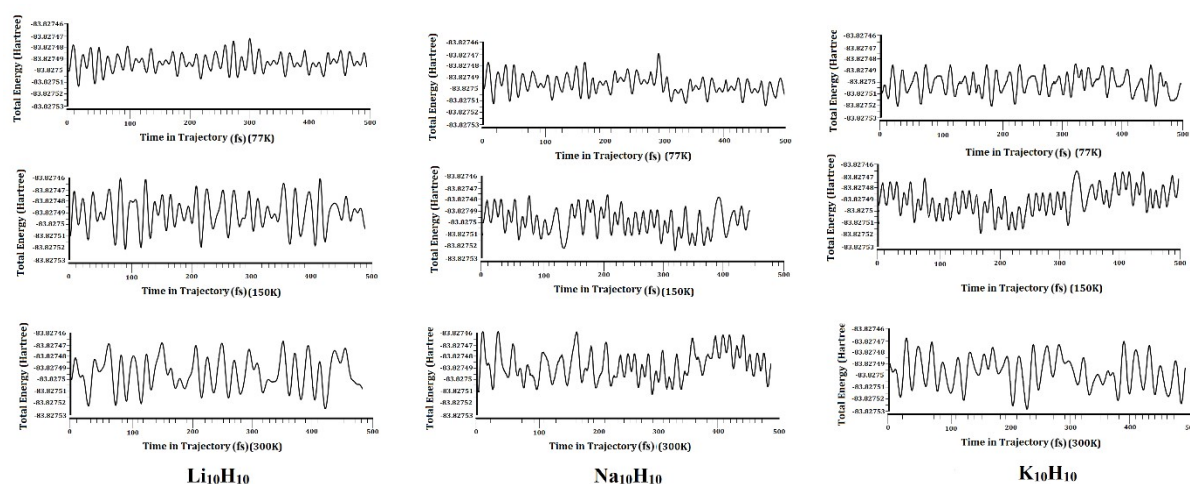


Figure S1: Evolution of energy of the M₁₀H₁₀ (M = Li, Na, K) cage structure at (a) 77 K, (b) 150 K and (c) 300K during 500 fs ab initio molecular dynamics simulations

Table S1: The atomization energy (kcal/mol) of the bare cages M₁₀H₁₀.

Compounds	Atomization energy (kcal/mol)
Li ₁₀ H ₁₀	-810.36
Na ₁₀ H ₁₀	-636.74
K ₁₀ H ₁₀	-592.87

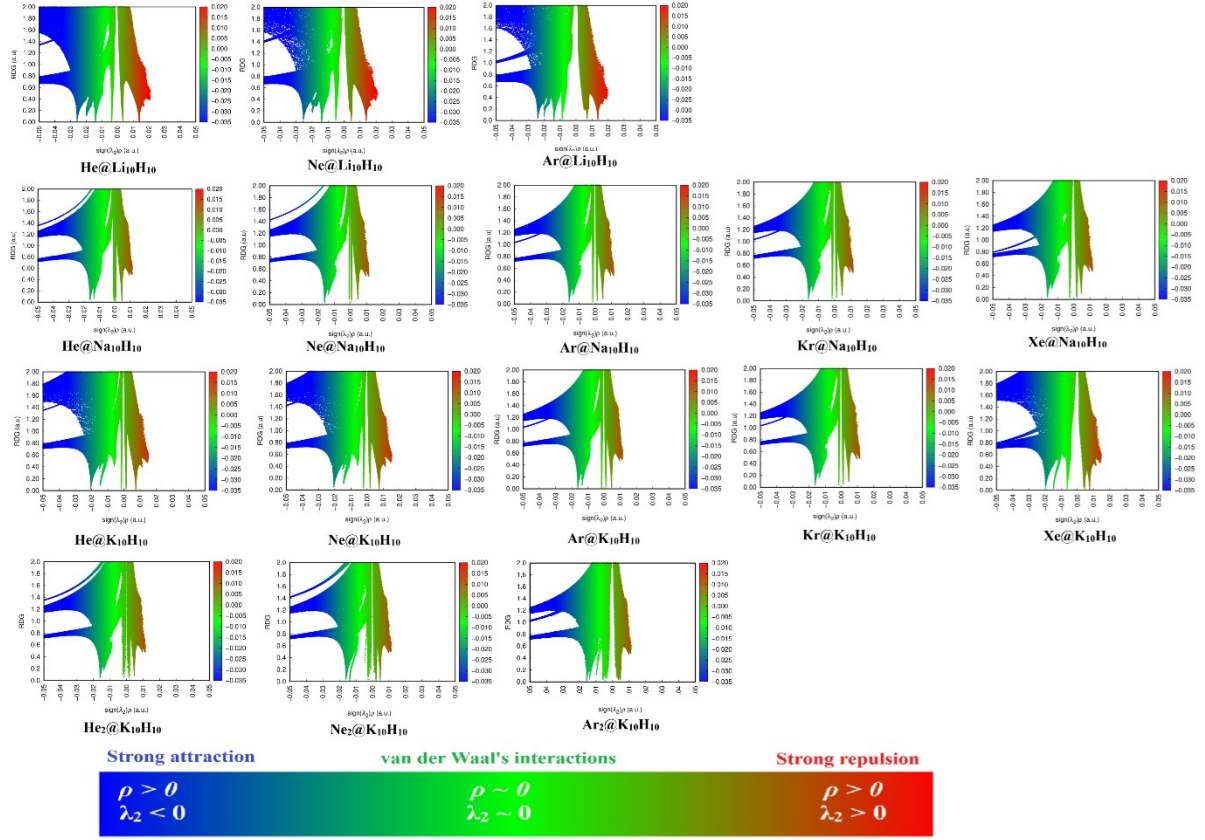


Figure S2: The reduced density gradient (RDG) color-filled scatter map of all the $\text{Ng}_n@M_{10}\text{H}_{10}$ complexes.

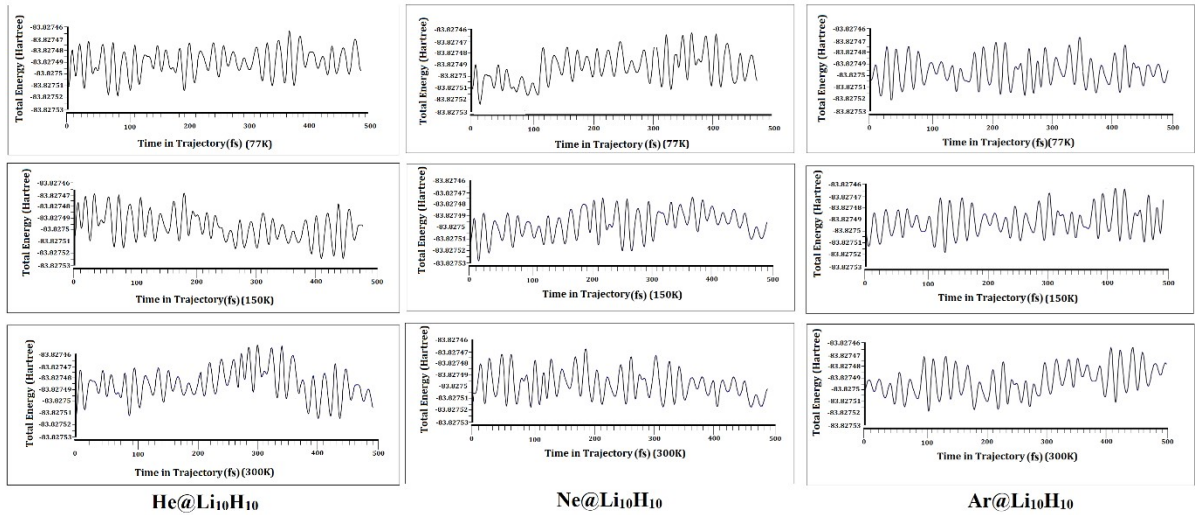


Figure S3. Evolution of energy of the $\text{Ng}@Li_{10}H_{10}$ cage structure at (a) 77 K, (b) 150 K and (c) 300K during 500 fs ab initio molecular dynamics simulations

Coordinates:**Li₁₀H₁₀**

3	2.359080000	1.498731000	-0.911700000
3	-1.025522000	-2.598154000	-0.912309000
3	-2.791198000	0.173624000	-0.911870000
3	-0.696793000	2.704747000	-0.911983000
1	-0.709303000	2.755393000	0.987017000
1	-2.843638000	0.176695000	0.987008000
1	2.403619000	1.528090000	0.985980000
3	2.154492000	-1.779775000	-0.910473000
1	-1.045412000	-2.646452000	0.986455000
1	2.193303000	-1.811787000	0.986427000
3	2.789028000	-0.172574000	0.911991000
3	-2.358849000	-1.498363000	0.911212000
3	-2.154836000	1.779273000	0.912237000
3	1.027390000	2.599808000	0.910703000
1	-2.195082000	1.812471000	-0.985731000
1	-2.401890000	-1.526295000	-0.986233000
1	1.046082000	2.646754000	-0.986750000
3	0.697008000	-2.707359000	0.912138000
1	0.711089000	-2.758160000	-0.986899000
1	2.841828000	-0.176583000	-0.987113000

He@Li₁₀H₁₀

3	1.840607000	-2.117295000	-0.910199000
3	-2.735953000	0.634658000	-0.911079000
3	-0.242569000	2.797222000	-0.908795000
3	2.586274000	1.095398000	-0.911377000
1	2.630712000	1.112241000	0.984949000

1	-0.245840000	2.839422000	0.987414000
1	1.870264000	-2.151637000	0.986658000
3	-1.446332000	-2.399185000	-0.911219000
1	-2.783257000	0.643444000	0.984838000
1	-1.470864000	-2.440316000	0.985402000
3	0.242759000	-2.795010000	0.912172000
3	-1.838432000	2.115408000	0.914108000
3	1.447479000	2.399840000	0.913746000
3	2.739746000	-0.633280000	0.911609000
1	1.470533000	2.442709000	-0.982936000
1	-1.869880000	2.154292000	-0.982692000
1	2.784354000	-0.644055000	-0.983934000
3	-2.590435000	-1.095456000	0.911607000
1	-2.632735000	-1.112940000	-0.984655000
1	0.247195000	-2.841963000	-0.983704000
2	-0.004956000	-0.004049000	-0.021532000

Ne@Li₁₀H₁₀

3	1.848936000	-2.123960000	-0.906781000
3	-2.745611000	0.636572000	-0.908003000
3	-0.243933000	2.808203000	-0.905353000
3	2.595732000	1.101096000	-0.907376000
1	2.637710000	1.117005000	0.989818000
1	-0.247461000	2.848277000	0.991763000
1	1.876913000	-2.157302000	0.990924000
3	-1.449991000	-2.408263000	-0.908485000
1	-2.790734000	0.644421000	0.988891000
1	-1.474081000	-2.448546000	0.988967000
3	0.244987000	-2.804984000	0.913847000

3	-1.845494000	2.122859000	0.915732000
3	1.451786000	2.409661000	0.915922000
3	2.749419000	-0.634208000	0.914041000
1	1.474469000	2.451284000	-0.981335000
1	-1.875797000	2.160832000	-0.981797000
1	2.792911000	-0.644184000	-0.982309000
3	-2.598597000	-1.100431000	0.912965000
1	-2.639422000	-1.116866000	-0.984256000
1	0.249770000	-2.849836000	-0.983069000
10	-0.002598000	-0.002472000	-0.014712000

Ar@Li₁₀H₁₀

3	1.532856000	2.422309000	0.904362000
3	-2.665636000	-1.059571000	0.905706000
3	0.184788000	-2.864840000	0.901935000
3	2.782197000	-0.710900000	0.903629000
1	2.817974000	-0.717948000	-0.988663000
1	0.186282000	-2.902205000	-0.989848000
1	1.554615000	2.455473000	-0.987823000
3	-1.830055000	2.203174000	0.904804000
1	-2.705222000	-1.073459000	-0.988206000
1	-1.858231000	2.235883000	-0.987201000
3	-0.185107000	2.861157000	-0.913017000
3	-1.533325000	-2.419861000	-0.912131000
3	1.829396000	-2.203863000	-0.914830000
3	2.670392000	1.061520000	-0.910723000
1	1.858870000	-2.240384000	0.978424000
1	-1.555132000	-2.458796000	0.980274000
1	2.708321000	1.075699000	0.981178000

3	-2.786211000	0.710927000	-0.912372000
1	-2.825065000	0.720305000	0.981386000
1	-0.187372000	2.903623000	0.980802000
18	0.000393000	0.000092000	0.009311000

Na₁₀H₁₀

11	0.256232000	3.343053000	-1.130521000
11	1.759777000	-2.851228000	-1.131544000
11	-2.172626000	-2.550738000	-1.131982000
11	-3.105516000	1.275935000	-1.129938000
1	-3.173195000	1.303073000	1.170154000
1	-2.221647000	-2.609640000	1.168956000
1	0.261259000	3.416417000	1.170420000
11	3.263436000	0.790631000	-1.129938000
1	1.798508000	-2.915540000	1.169103000
1	3.335131000	0.807000000	1.170035000
11	2.171563000	2.551778000	1.131899000
11	-0.255656000	-3.339016000	1.129995000
11	-3.268029000	-0.792386000	1.130443000
11	-1.757714000	2.850335000	1.131338000
1	-3.340777000	-0.808673000	-1.169706000
1	-0.260708000	-3.411466000	-1.171240000
1	-1.796791000	2.913993000	-1.169560000
11	3.108533000	-1.278362000	1.130341000
1	3.177134000	-1.305342000	-1.169905000
1	2.221081000	2.610167000	-1.169269000

He@Na₁₀H₁₀

11	1.457033000	3.018706000	-1.132082000
----	-------------	-------------	--------------

11	0.596852000	-3.298897000	-1.131348000
11	-2.957935000	-1.589532000	-1.130602000
11	-2.423885000	2.319396000	-1.131279000
1	-2.476597000	2.370283000	1.169372000
1	-3.021925000	-1.622574000	1.169641000
1	1.489349000	3.085613000	1.168630000
11	3.327057000	-0.453516000	-1.130931000
1	0.609998000	-3.370658000	1.170094000
1	3.398518000	-0.462070000	1.169395000
11	2.956905000	1.588407000	1.130069000
11	-1.457187000	-3.018985000	1.131766000
11	-3.326030000	0.452833000	1.130109000
11	-0.596912000	3.300056000	1.131586000
1	-3.396720000	0.461610000	-1.169835000
1	-1.489258000	-3.085482000	-1.169455000
1	-0.610097000	3.371089000	-1.169360000
11	2.423727000	-2.318881000	1.131915000
1	2.476649000	-2.370234000	-1.169261000
1	3.020697000	1.621384000	-1.170515000
2	0.001754000	0.002784000	0.005025000

Ne@Na₁₀H₁₀

11	-0.293663000	3.325987000	-1.133412000
11	2.201590000	-2.524536000	-1.133300000
11	-1.728892000	-2.869181000	-1.131658000
11	-3.275385000	0.755361000	-1.133237000
1	-3.350476000	0.771806000	1.166346000
1	-1.766027000	-2.928789000	1.169548000
1	-0.298314000	3.397980000	1.168311000

11	3.098549000	1.310066000	-1.132558000
1	2.250464000	-2.578761000	1.168900000
1	3.164812000	1.339061000	1.167298000
11	1.728023000	2.864975000	1.129152000
11	0.292171000	-3.324244000	1.131194000
11	-3.096306000	-1.309545000	1.128179000
11	-2.203869000	2.526671000	1.130932000
1	-3.160163000	-1.338067000	-1.172094000
1	0.297930000	-3.399645000	-1.170663000
1	-2.253419000	2.584240000	-1.171433000
11	3.280066000	-0.754255000	1.129963000
1	3.349473000	-0.771220000	-1.171154000
1	1.762433000	2.923805000	-1.172512000
10	-0.002183000	-0.001471000	0.017963000

Ar@Na₁₀H₁₀

11	1.161651000	3.147928000	-1.130298000
11	0.913144000	-3.230130000	-1.130238000
11	-2.793491000	-1.867270000	-1.129998000
11	-2.641740000	2.077837000	-1.130718000
1	-2.697036000	2.121592000	1.169821000
1	-2.852184000	-1.905549000	1.169665000
1	1.185275000	3.213816000	1.169451000
11	3.357644000	-0.130388000	-1.131109000
1	0.932121000	-3.296604000	1.169635000
1	3.428795000	-0.133091000	1.168353000
11	2.793773000	1.866289000	1.131054000
11	-1.161027000	-3.146177000	1.131695000
11	-3.357068000	0.130859000	1.131047000

11	-0.913235000	3.225778000	1.131059000
1	-3.428440000	0.132874000	-1.168266000
1	-1.185567000	-3.215441000	-1.168580000
1	-0.932058000	3.294810000	-1.168729000
11	2.639061000	-2.075982000	1.131033000
1	2.694527000	-2.121436000	-1.170148000
1	2.853689000	1.907531000	-1.169278000
18	0.000836000	0.000850000	-0.002262000

Kr@Na₁₀H₁₀

11	1.867271000	2.807387000	-1.128100000
11	0.141803000	-3.364936000	-1.130027000
11	-3.166639000	-1.177986000	-1.128472000
11	-2.100274000	2.642800000	-1.129333000
1	-2.138621000	2.691691000	1.167679000
1	-3.224181000	-1.199861000	1.169534000
1	1.901897000	2.859385000	1.168889000
11	3.250372000	-0.904630000	-1.131215000
1	0.145924000	-3.431794000	1.167423000
1	3.315994000	-0.924604000	1.166135000
11	3.159964000	1.173795000	1.129555000
11	-1.860824000	-2.800650000	1.130556000
11	-3.243277000	0.902860000	1.130499000
11	-0.142418000	3.353071000	1.130429000
1	-3.310998000	0.921664000	-1.167404000
1	-1.899367000	-2.857120000	-1.166920000
1	-0.145394000	3.422913000	-1.167252000
11	2.093191000	-2.636537000	1.128174000
1	2.132752000	-2.686737000	-1.169980000

1	3.222890000	1.199195000	-1.167678000
36	0.000229000	0.001621000	-0.000643000

Xe@Na₁₀H₁₀

11	3.326318000	0.713081000	-1.123824000
11	-2.269690000	-2.528926000	-1.125136000
11	-3.109244000	1.375797000	-1.125379000
11	0.350165000	3.379650000	-1.125707000
1	0.354737000	3.444049000	1.170526000
1	-3.167355000	1.401793000	1.169455000
1	3.384263000	0.725218000	1.170660000
11	1.705336000	-2.937165000	-1.126237000
1	-2.310615000	-2.575295000	1.169869000
1	1.736657000	-2.993686000	1.169399000
11	3.105266000	-1.376062000	1.129257000
11	-3.321527000	-0.712385000	1.129844000
11	-1.703820000	2.934811000	1.128605000
11	2.266304000	2.525925000	1.130657000
1	-1.733547000	2.988619000	-1.165139000
1	-3.383724000	-0.725859000	-1.164459000
1	2.310910000	2.573983000	-1.164147000
11	-0.347933000	-3.375261000	1.128806000
1	-0.354671000	-3.440351000	-1.166029000
1	3.165939000	-1.400900000	-1.164908000
54	-0.000287000	0.000154000	-0.004722000

K₁₀H₁₀

19	0.147990000	4.109944000	-1.375688000
19	2.301497000	-3.408141000	-1.376757000

19	-2.537700000	-3.233740000	-1.377773000
19	-3.875167000	1.410637000	-1.375777000
1	-3.862850000	1.403302000	1.275341000
1	-2.531008000	-3.221791000	1.272957000
1	0.146089000	4.094826000	1.275202000
19	3.968909000	1.131260000	-1.373863000
1	2.291703000	-3.394954000	1.273229000
1	3.950796000	1.124848000	1.276889000
19	2.536991000	3.235067000	1.377729000
19	-0.147367000	-4.102092000	1.376358000
19	-3.978391000	-1.134551000	1.373161000
19	-2.298589000	3.406080000	1.377136000
1	-3.959849000	-1.128522000	-1.278065000
1	-0.145311000	-4.088594000	-1.274779000
1	-2.288335000	3.393726000	-1.273224000
19	3.881814000	-1.414431000	1.375562000
1	3.869281000	-1.407691000	-1.275856000
1	2.529716000	3.224220000	-1.273380000

He@K₁₀H₁₀

19	1.596218000	3.788766000	1.372993000
19	-3.524163000	-2.128404000	1.373516000
19	0.941152000	-3.980800000	1.379939000
19	4.120216000	-0.339963000	1.374071000
1	4.102437000	-0.339952000	-1.278054000
1	0.938506000	-3.970587000	-1.273460000
1	1.588683000	3.771620000	-1.279442000
19	-3.122283000	2.683176000	1.378936000
1	-3.508743000	-2.116176000	-1.278285000

1	-3.116236000	2.673797000	-1.274658000
19	-0.940429000	3.982226000	-1.379518000
19	-1.591252000	-3.779188000	-1.374154000
19	3.125380000	-2.682062000	-1.376885000
19	3.526271000	2.131944000	-1.375473000
1	3.115315000	-2.669687000	1.276846000
1	-1.587867000	-3.769491000	1.278579000
1	3.512407000	2.124601000	1.275814000
19	-4.125863000	0.346050000	-1.373042000
1	-4.103276000	0.342724000	1.279174000
1	-0.934313000	3.969858000	1.274035000
2	-0.053299000	-0.214925000	-0.003907000

Ne@K₁₀H₁₀

19	-1.552480000	-3.802374000	1.376365000
19	3.495766000	2.166035000	1.376415000
19	-0.982709000	3.986838000	1.376254000
19	-4.109291000	0.299586000	1.375534000
1	-4.096107000	0.297368000	-1.277421000
1	-0.979191000	3.972193000	-1.276263000
1	-1.547779000	-3.790145000	-1.276689000
19	3.144256000	-2.650374000	1.376504000
1	3.483037000	2.157007000	-1.275996000
1	3.134646000	-2.642056000	-1.276255000
19	0.981454000	-3.983751000	-1.376638000
19	1.551339000	3.801366000	-1.376268000
19	-3.143944000	2.650182000	-1.376629000
19	-3.498973000	-2.168247000	-1.376027000
1	-3.134181000	2.642416000	1.276249000

1	1.546267000	3.789991000	1.276781000
1	-3.485149000	-2.158889000	1.276468000
19	4.111980000	-0.300054000	-1.375448000
1	4.098563000	-0.298339000	1.277706000
1	0.978267000	-3.970278000	1.276058000
10	0.005108000	0.001585000	-0.000182000

Ar@K₁₀H₁₀

19	0.872083000	4.009804000	-1.374699000
19	1.655156000	-3.747031000	-1.377570000
19	-3.063070000	-2.728228000	-1.376846000
19	-3.548016000	2.064583000	-1.378444000
1	-3.541984000	2.058545000	1.273797000
1	-3.055986000	-2.721001000	1.275361000
1	0.868617000	3.998851000	1.278806000
19	4.090463000	0.411329000	-1.375371000
1	1.649110000	-3.738913000	1.274592000
1	4.078214000	0.409689000	1.277062000
19	3.062186000	2.730485000	1.377468000
19	-0.870100000	-4.002063000	1.375317000
19	-4.100586000	-0.412259000	1.376000000
19	-1.652727000	3.745909000	1.378167000
1	-4.088296000	-0.411083000	-1.276859000
1	-0.867048000	-3.992662000	-1.278466000
1	-1.646208000	3.737741000	-1.274366000
19	3.553516000	-2.068899000	1.379151000
1	3.547043000	-2.062965000	-1.273366000
1	3.055009000	2.724131000	-1.275113000
18	0.001240000	-0.003962000	-0.003430000

Kr@K₁₀H₁₀

19	-0.041880000	4.108233000	-1.375526000
19	2.394104000	-3.289071000	-1.372483000
19	-2.431612000	-3.315872000	-1.375109000
19	-3.930845000	1.262148000	-1.370955000
1	-3.914828000	1.256278000	1.282869000
1	-2.428995000	-3.311644000	1.279041000
1	-0.043210000	4.106122000	1.278199000
19	3.874759000	1.287852000	-1.369094000
1	2.387388000	-3.284260000	1.280602000
1	3.859996000	1.284827000	1.284473000
19	2.365462000	3.327564000	1.382131000
19	-0.015705000	-4.076692000	1.382956000
19	-3.932874000	-1.275410000	1.379181000
19	-2.449796000	3.321716000	1.380672000
1	-3.922428000	-1.269495000	-1.274849000
1	-0.014579000	-4.059555000	-1.269351000
1	-2.443542000	3.310163000	-1.272727000
19	3.886092000	-1.246022000	1.380673000
1	3.884715000	-1.243374000	-1.272968000
1	2.359662000	3.313600000	-1.270704000
36	0.156650000	-0.057976000	-0.023641000

Xe@K₁₀H₁₀

19	-0.258198000	4.083090000	1.375428000
19	-2.193140000	-3.445908000	1.378683000
19	2.610481000	-3.145619000	1.376725000
19	3.812105000	1.505040000	1.376241000

1	3.806913000	1.501775000	-1.277475000
1	2.606053000	-3.136915000	-1.277890000
1	-0.254151000	4.071417000	-1.278511000
19	-3.974637000	1.018262000	1.373136000
1	-2.189211000	-3.440400000	-1.276326000
1	-3.960855000	1.013059000	-1.280368000
19	-2.606388000	3.146943000	-1.381300000
19	0.257312000	-4.072948000	-1.380046000
19	3.986158000	-1.019868000	-1.375276000
19	2.194059000	3.448089000	-1.379815000
1	3.973974000	-1.017375000	1.278836000
1	0.255970000	-4.063121000	1.273933000
1	2.184649000	3.437859000	1.274136000
19	-3.820234000	-1.509939000	-1.376988000
1	-3.811299000	-1.504236000	1.277373000
1	-2.604490000	3.142041000	1.273393000
54	-0.002785000	-0.002589000	0.004887000

He₂@K₁₀H₁₀

19	4.365353000	-0.667259000	-1.360916000
19	-3.898347000	-1.843388000	-1.358956000
19	-2.996821000	2.805081000	-1.373563000
19	1.896686000	3.408177000	-1.373961000
1	1.893752000	3.394455000	1.278051000
1	-2.994726000	2.800220000	1.277025000
1	4.353867000	-0.655278000	1.284981000
19	0.624104000	-3.731246000	-1.374258000
1	-3.883402000	-1.821861000	1.288789000

1	0.624278000	-3.699523000	1.277755000
19	2.995475000	-2.806520000	1.375429000
19	-4.378810000	0.670987000	1.362387000
19	-0.625761000	3.720155000	1.377760000
19	3.904383000	1.846520000	1.360209000
1	-0.624364000	3.695565000	-1.274648000
1	-4.360063000	0.656592000	-1.284620000
1	3.892517000	1.830697000	-1.288422000
19	-1.895644000	-3.407248000	1.378152000
1	-1.894948000	-3.401010000	-1.274594000
1	2.990119000	-2.802777000	-1.275301000
2	-1.243061000	0.012214000	-0.068966000
2	1.333674000	0.034283000	-0.052234000

Ne₂@K₁₀H₁₀

19	-0.012583000	-3.522964000	-1.385401000
19	-2.483510000	3.067749000	-1.366830000
19	2.506682000	3.065612000	-1.367032000
19	4.304263000	-1.286120000	-1.373047000
1	4.294714000	-1.282942000	1.272966000
1	2.510103000	3.048839000	1.282568000
1	-0.010655000	-3.516608000	1.265601000
19	-4.315559000	-1.264518000	-1.370370000
1	-2.484732000	3.050719000	1.283543000
1	-4.301984000	-1.258411000	1.275288000
19	-2.505727000	-3.060005000	1.370545000
19	0.012516000	3.526215000	1.388145000
19	4.311190000	1.260807000	1.370233000
19	2.486862000	-3.073322000	1.366621000

1	4.295619000	1.257026000	-1.275198000
1	0.011742000	3.520630000	-1.262595000
1	2.486174000	-3.055358000	-1.283005000
19	-4.306494000	1.285136000	1.370648000
1	-4.294789000	1.280034000	-1.275316000
1	-2.509253000	-3.045904000	-1.279306000
10	1.399009000	0.000423000	0.012939000
10	-1.394220000	0.002452000	-0.020069000

Ar₂@K₁₀H₁₀

19	-0.017442000	-3.104302000	-1.423250000
19	-2.560284000	3.006576000	-1.314516000
19	2.542000000	2.995570000	-1.340718000
19	4.473010000	-1.276785000	-1.398761000
1	4.478058000	-1.295536000	1.246183000
1	2.585624000	2.970162000	1.309770000
1	0.008220000	-3.114425000	1.223734000
19	-4.503400000	-1.273944000	-1.354133000
1	-2.543513000	2.945036000	1.334208000
1	-4.443626000	-1.281007000	1.289436000
19	-2.541978000	-2.995270000	1.340834000
19	0.017402000	3.103497000	1.423340000
19	4.503500000	1.274080000	1.354170000
19	2.560298000	-3.006384000	1.314394000
1	4.443450000	1.281168000	-1.289373000
1	-0.008187000	3.113745000	-1.223445000
1	2.543409000	-2.944992000	-1.334358000
19	-4.473239000	1.276987000	1.398635000
1	-4.477967000	1.295663000	-1.246262000

1	-2.585580000	-2.970120000	-1.309657000
18	1.595845000	0.000274000	0.121670000
18	-1.595698000	-0.000285000	-0.121677000