

Supplementary Information

for

What causes the weakest host to act as the strongest one?

**A theoretical study on host-guest chemistry of five
azacryptands and fluoride anion**

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Table S1. Computed and experimental distances (Å) for five complexes studied here^a.

Complex	F...H1	F...H2	F...H3	F...H4	F...H5	F...H6	rms
[F⊂H ₆ 1] ⁵⁺	1.688	2.555	1.537	1.724	–	–	–
	<i>1.678</i>	<i>2.462</i>	<i>1.545</i>	<i>1.706</i>	–	–	–
	–	–	–	–	–	–	–
[F⊂H ₆ 2] ⁵⁺	1.653	1.683	1.670	–	–	–	–
	<i>1.652</i>	<i>1.641</i>	<i>1.675</i>	–	–	–	–
	–	–	–	–	–	–	–
[F⊂H ₆ 3] ⁵⁺	2.678	2.777	2.980	1.614	1.705	1.714	0.209
	<i>2.670</i>	<i>2.760</i>	<i>2.952</i>	<i>1.611</i>	<i>1.682</i>	<i>1.696</i>	<i>0.199</i>
	2.510	2.392	2.830	1.861	1.661	1.693	–
[F⊂H ₆ 4] ⁵⁺	2.028	1.977	1.976	1.976	2.016	1.992	0.113
	<i>2.008</i>	<i>1.956</i>	<i>1.994</i>	<i>1.958</i>	<i>1.956</i>	<i>1.970</i>	<i>0.132</i>
	2.071	1.949	1.904	1.998	2.223	1.830	–
	F...H1	F...H2	F...C1	F...C2	F...C3		
[F⊂H ₂ 5] ⁵⁺	1.537	1.537	2.611	2.612	2.608	–	0.108
	<i>1.539</i>	<i>1.541</i>	<i>2.574</i>	<i>2.566</i>	<i>2.569</i>	–	<i>0.108</i>
	1.676	1.735	2.609	2.587	2.596	–	–

^a The data obtained at the PBE/TZVP level are given as plain text, those for the B3P86/TZVP level are in italic and experimental data are in bold.

Table S2. Calculated ΔG_{gas}^0 , ΔG_{solv}^0 and ΔG_{aq}^0 values for formation of studied complexes in water^a.

Complex	ΔG_{gas}^0	ΔG_{solv}^0	ΔG_{aq}^0
[F⊂H ₆ 1] ⁵⁺	-421.56	394.62	-26.94
	<i>-418.92</i>	382.10	<i>-36.82</i>
[F⊂H ₆ 2] ⁵⁺	-462.67	422.12	-40.55
	<i>-460.56</i>	<i>418.81</i>	<i>-41.75</i>
[F⊂H ₆ 3] ⁵⁺	-464.57	419.28	-45.29
	<i>-463.14</i>	<i>414.51</i>	<i>-48.63</i>
[F⊂H ₆ 4] ⁵⁺	-490.31	431.53	-58.78
	<i>-489.53</i>	<i>430.75</i>	<i>-58.78</i>
[F⊂H ₂ 5] ⁴⁺	-446.28	364.92	-81.36
	<i>-446.23</i>	<i>365.43</i>	<i>-80.80</i>

^a The data obtained at the PBE/TZVP level are given as plain text, those for the B3P86/TZVP level are in italic. Solvation energies have been calculated using DPCM model.

Cartesian coordinate representation of the optimized molecular structures of H_61^{6+} , H_62^{6+} , H_63^{6+} , H_64^{6+} , H_25^{5+} , H_6222^{6+} , $[F\subset H_61]^{5+}$, $[F\subset H_62]^{5+}$, $[F\subset H_63]^{5+}$, $[F\subset H_64]^{5+}$ and $[F\subset H_25]^{4+}$ at PBE/TZVP level of theory:

H_61^{6+}			
N	-3.277354000	1.509348000	0.398586000
C	-3.350902000	1.335985000	1.876524000
C	-3.111808000	-0.127852000	2.305394000
N	-2.761529000	-0.250587000	3.775443000
C	-2.507118000	-1.667153000	4.313570000
C	-1.440524000	-2.455143000	3.558669000
O	-0.150003000	-1.818216000	3.545749000
C	4.225706000	-0.212219000	-0.619192000
C	3.533865000	1.119673000	-0.980587000
N	4.515925000	2.247613000	-1.238630000
C	3.912591000	3.569005000	-1.750956000
C	3.194510000	4.418818000	-0.718375000
O	1.877919000	3.905394000	-0.408370000
C	1.225779000	4.630049000	0.651660000
C	0.016270000	5.454729000	0.226637000
N	-1.182735000	4.656404000	-0.322000000
C	-1.623565000	3.442150000	0.474517000
C	-3.014782000	2.932938000	0.040763000
N	3.240906000	-1.322088000	-0.459382000
C	3.776966000	-2.426094000	0.394771000
C	4.031816000	-2.129313000	1.873475000
N	2.800784000	-1.803838000	2.727314000
C	2.034128000	-2.968660000	3.344472000
C	0.910966000	-2.488067000	4.264414000
C	-4.559043000	1.082582000	-0.245990000
C	-4.479734000	0.747382000	-1.742977000
N	-3.998575000	-0.665015000	-2.044360000
C	-3.670947000	-0.951757000	-3.507059000
C	-3.022742000	-2.316107000	-3.670397000
O	-1.783617000	-2.334545000	-2.915433000
C	-1.227958000	-3.647402000	-2.702328000
C	0.023376000	-3.940688000	-3.520666000
N	1.185141000	-2.962809000	-3.284951000
C	1.651828000	-2.756992000	-1.855336000
C	2.910068000	-1.864272000	-1.809217000
H	-3.088337000	3.004778000	-1.056031000
H	-3.797181000	3.602742000	0.451115000
H	-0.859335000	2.669086000	0.319425000
H	-1.609312000	3.757323000	1.526300000
H	-0.967272000	4.375341000	-1.290656000

H	-1.966237000	5.329388000	-0.396226000
H	0.260417000	6.185035000	-0.558241000
H	-0.358597000	6.009117000	1.100150000
H	1.912002000	5.350825000	1.127947000
H	0.948834000	3.906379000	1.435771000
H	3.797384000	4.512216000	0.204654000
H	3.125188000	5.430095000	-1.157757000
H	4.768476000	4.146889000	-2.131976000
H	3.270112000	3.310974000	-2.603450000
H	5.209757000	1.944135000	-1.944561000
H	5.070780000	2.448569000	-0.389079000
H	2.863740000	1.462734000	-0.183175000
H	2.945274000	1.036027000	-1.903897000
H	4.995094000	-0.465178000	-1.376414000
H	4.764691000	-0.084322000	0.330223000
H	3.080556000	-3.273708000	0.316486000
H	4.747425000	-2.801853000	0.011086000
H	4.726154000	-1.291050000	2.020040000
H	4.507999000	-3.009719000	2.328346000
H	3.120940000	-1.210016000	3.509298000
H	2.147083000	-1.232067000	2.170604000
H	1.660627000	-3.593639000	2.523278000
H	2.760786000	-3.550647000	3.931173000
H	1.303106000	-1.795542000	5.029463000
H	0.536633000	-3.372868000	4.804264000
H	-1.747270000	-2.632038000	2.514675000
H	-1.400811000	-3.444412000	4.044317000
H	-2.244616000	-1.530307000	5.372780000
H	-3.465515000	-2.205281000	4.266449000
H	-3.519505000	0.155461000	4.352380000
H	-1.921534000	0.313085000	3.979667000
H	-3.992899000	-0.765508000	2.150677000
H	-2.264795000	-0.542286000	1.744503000
H	-4.308204000	1.709697000	2.290244000
H	-2.555885000	1.951930000	2.324815000
H	-5.334966000	1.865329000	-0.139972000
H	-4.958137000	0.214125000	0.300648000
H	-3.812671000	1.422856000	-2.293852000
H	-5.478872000	0.835131000	-2.193069000
H	-4.721924000	-1.335648000	-1.736166000
H	-3.144783000	-0.872677000	-1.502461000
H	-4.606055000	-0.901225000	-4.082873000
H	-3.006348000	-0.144955000	-3.843605000
H	-3.691978000	-3.122372000	-3.320523000
H	-2.847377000	-2.474505000	-4.748131000
H	-1.022473000	-3.748394000	-1.624566000
H	-1.950446000	-4.440290000	-2.959083000
H	0.395177000	-4.946910000	-3.276069000
H	-0.166707000	-3.904127000	-4.603393000
H	0.911759000	-2.054616000	-3.691519000
H	1.975337000	-3.303115000	-3.860959000
H	0.821995000	-2.287958000	-1.311352000

H	1.828537000	-3.761333000	-1.447966000
H	3.771742000	-2.421288000	-2.230490000
H	2.737615000	-1.003216000	-2.473685000

H₆2⁶⁺

N	2.859249000	0.354092000	0.820087000
C	3.413133000	1.688681000	1.206862000
C	2.466317000	2.895786000	1.066880000
N	2.442601000	3.556129000	-0.317493000
C	1.175498000	4.326168000	-0.702144000
C	-0.022563000	3.381913000	-0.906897000
C	-1.228098000	4.084835000	-1.555997000
N	-2.484800000	3.209954000	-1.508574000
C	-2.487764000	1.945335000	-2.376151000
C	-3.422330000	0.817849000	-1.897161000
C	1.735807000	-0.108758000	1.667332000
C	1.915874000	-0.157951000	3.216988000
N	0.807475000	-0.963765000	3.910165000
C	-0.638941000	-0.457883000	3.774229000
C	-1.646338000	-1.621177000	3.736778000
C	-3.133895000	-1.244275000	3.646580000
N	-3.643644000	-0.675413000	2.304741000
C	-3.615839000	-1.604507000	1.095179000
C	-3.949348000	-0.935451000	-0.251128000
C	3.955515000	-0.653167000	0.681022000
C	3.633956000	-1.912527000	-0.145435000
N	3.658478000	-1.716846000	-1.657983000
C	3.158846000	-2.886315000	-2.533568000
C	1.675273000	-3.273057000	-2.421409000
C	0.656165000	-2.288972000	-3.023527000
N	-0.784727000	-2.811016000	-2.887672000
C	-1.904630000	-1.778091000	-2.696233000
C	-1.731670000	-0.951582000	-1.383528000
N	-2.860996000	-0.131492000	-0.887132000
H	4.321353000	1.861775000	0.607787000
H	3.774214000	1.701275000	2.252398000
H	2.781334000	3.685699000	1.762884000
H	1.428456000	2.639222000	1.308876000
H	2.637720000	2.853320000	-1.046475000
H	3.231474000	4.227314000	-0.367838000
H	1.428380000	4.872255000	-1.623797000
H	0.999694000	5.068373000	0.089683000
H	-0.336104000	2.968544000	0.066923000
H	0.297091000	2.538052000	-1.542004000
H	-1.053640000	4.336451000	-2.611993000
H	-1.492828000	5.014107000	-1.028771000
H	-3.280124000	3.806149000	-1.804198000
H	-2.680869000	2.963955000	-0.526563000
H	-1.445074000	1.615445000	-2.449873000

H	-2.800763000	2.276317000	-3.376180000
H	-3.768596000	0.297748000	-2.809967000
H	-4.340350000	1.254769000	-1.473110000
H	1.471777000	-1.121661000	1.320577000
H	0.865483000	0.525143000	1.435062000
H	1.898842000	0.837165000	3.681429000
H	2.854812000	-0.647783000	3.514103000
H	1.045319000	-1.006475000	4.919223000
H	0.858231000	-1.946695000	3.594265000
H	-0.663842000	0.142399000	2.855702000
H	-0.816674000	0.211574000	4.627883000
H	-1.580193000	-2.191325000	4.680563000
H	-1.381246000	-2.339068000	2.941921000
H	-3.414380000	-0.498546000	4.405880000
H	-3.741527000	-2.141396000	3.833864000
H	-3.153343000	0.201018000	2.075888000
H	-4.628597000	-0.402997000	2.477859000
H	-4.363906000	-2.385141000	1.297264000
H	-2.631019000	-2.088294000	1.095011000
H	-4.824940000	-0.279077000	-0.125540000
H	-4.312739000	-1.749762000	-0.906158000
H	4.317131000	-1.022766000	1.659256000
H	4.828843000	-0.143797000	0.244111000
H	2.653667000	-2.340674000	0.098604000
H	4.390191000	-2.681023000	0.072004000
H	4.641766000	-1.559173000	-1.945270000
H	3.160193000	-0.848465000	-1.899596000
H	3.775879000	-3.750675000	-2.248519000
H	3.434434000	-2.617254000	-3.564597000
H	1.415389000	-3.509695000	-1.375416000
H	1.616928000	-4.234352000	-2.962391000
H	0.828085000	-2.125645000	-4.097050000
H	0.672754000	-1.313733000	-2.520198000
H	-0.828863000	-3.501892000	-2.119879000
H	-1.015244000	-3.358474000	-3.738449000
H	-2.837164000	-2.361319000	-2.704438000
H	-1.894751000	-1.153247000	-3.599444000
H	-0.865856000	-0.281207000	-1.503240000
H	-1.462066000	-1.649093000	-0.573073000

H₆3⁶⁺

N	-2.361646000	3.709922000	-0.591737000
H	-2.787336000	4.655401000	-0.636688000
H	-2.080167000	3.499030000	-1.561284000
N	-1.981621000	-2.003279000	3.492015000
H	-1.923698000	-2.909936000	3.000240000
H	-2.247060000	-2.250594000	4.464856000
N	-2.498779000	-2.163935000	-3.165325000
H	-2.466647000	-1.317446000	-3.756397000
H	-2.860465000	-2.907026000	-3.793914000

N	2.275299000	3.791216000	-0.497602000
H	3.085499000	4.113053000	-1.058470000
H	2.486974000	4.104654000	0.466179000
N	2.564675000	-1.613616000	2.571684000
H	1.859913000	-1.513171000	1.828017000
H	2.958994000	-2.564891000	2.476937000
N	2.061346000	-1.545293000	-2.896007000
H	1.410605000	-0.988042000	-2.325449000
H	2.256330000	-0.992294000	-3.747763000
N	3.346056000	0.066163000	-0.193600000
C	-3.188603000	1.274030000	-0.019567000
C	-3.289710000	0.390503000	-1.112126000
H	-3.530692000	0.792792000	-2.102068000
C	-3.228764000	-1.007314000	-0.930387000
C	-3.102288000	-1.513120000	0.378300000
H	-3.183562000	-2.594547000	0.528761000
C	-3.015834000	-0.658537000	1.494227000
C	-3.045085000	0.729941000	1.272995000
H	-3.067074000	1.401957000	2.136012000
C	-3.508203000	2.756808000	-0.167405000
H	-4.293208000	2.914003000	-0.922492000
H	-3.883070000	3.167103000	0.780467000
C	-3.153405000	-1.175294000	2.921451000
H	-3.293935000	-0.343774000	3.624642000
H	-4.033490000	-1.831558000	3.013437000
C	-3.561188000	-1.980363000	-2.055078000
H	-3.742371000	-2.987315000	-1.656660000
H	-4.474145000	-1.672161000	-2.588482000
C	-1.156342000	3.757110000	0.336661000
H	-0.768328000	2.730451000	0.372280000
H	-1.574328000	3.992931000	1.325393000
C	-0.088183000	4.820829000	-0.001680000
H	-0.590263000	5.743768000	-0.344198000
H	0.352888000	5.140061000	0.958838000
C	1.041887000	4.570936000	-1.016586000
H	0.732659000	4.062384000	-1.940605000
H	1.445880000	5.550790000	-1.312096000
C	-0.630059000	-1.316510000	3.495807000
H	-0.745382000	-0.422276000	4.125405000
H	-0.474509000	-0.986661000	2.456701000
C	0.515768000	-2.202819000	4.019903000
H	0.348469000	-2.434805000	5.085168000
H	0.545581000	-3.181851000	3.510041000
C	1.894610000	-1.519215000	3.952904000
H	1.841914000	-0.451766000	4.208715000
H	2.588931000	-1.992800000	4.660734000
C	-1.104563000	-2.529700000	-2.695478000
H	-1.200327000	-3.493629000	-2.174914000
H	-0.847829000	-1.762135000	-1.948601000
C	-0.069480000	-2.629162000	-3.833319000
H	-0.113226000	-1.754112000	-4.505969000
H	-0.302107000	-3.496987000	-4.472751000

C	1.373408000	-2.846401000	-3.336474000
H	1.424873000	-3.540113000	-2.485593000
H	1.994407000	-3.263556000	-4.141548000
C	2.199717000	2.273774000	-0.569677000
H	2.017704000	2.046388000	-1.629683000
H	1.320530000	1.967482000	0.011838000
C	3.459531000	1.552325000	-0.046136000
H	4.366911000	1.936156000	-0.551444000
H	3.584497000	1.790385000	1.020431000
C	3.677312000	-0.599848000	2.297802000
H	3.285685000	0.376594000	2.612931000
H	4.505134000	-0.854146000	2.976106000
C	4.191757000	-0.609048000	0.852426000
H	4.363011000	-1.650026000	0.534877000
H	5.201330000	-0.155232000	0.887646000
C	3.370617000	-1.680584000	-2.111913000
H	4.108705000	-2.091131000	-2.816131000
H	3.195376000	-2.437805000	-1.336286000
C	3.872526000	-0.340625000	-1.543905000
H	4.977106000	-0.400484000	-1.522988000
H	3.653439000	0.462355000	-2.266668000

H₆4⁶⁺

C	4.012422000	-0.490144000	-0.253606000
C	3.364042000	-0.450586000	-1.645215000
C	3.517550000	-1.344002000	2.168876000
N	3.381554000	-1.561161000	0.658419000
C	2.597556000	-2.205940000	3.045473000
N	2.019545000	0.215538000	-1.707030000
C	2.157765000	1.705269000	-1.809613000
C	1.176300000	-0.331965000	-2.813778000
N	1.235124000	-1.585645000	3.419430000
C	0.271084000	-1.486245000	-2.314953000
C	1.046046000	2.390985000	-0.981929000
N	0.989778000	3.913547000	-1.040338000
N	-0.790332000	-1.924799000	-3.320265000
C	0.251879000	-1.328976000	2.282079000
C	-1.856350000	-2.949557000	-2.846329000
C	0.142415000	4.635761000	0.034464000
C	-2.413954000	-2.835501000	-1.421781000
C	-1.018120000	-0.552630000	2.708710000
N	-1.950306000	-0.301519000	1.562392000
C	-1.391457000	4.475656000	-0.009807000
C	-1.716177000	2.059842000	0.916985000
N	-3.418512000	-1.726969000	-1.140845000
C	-2.922909000	-1.440636000	1.477258000
N	-2.058237000	3.539394000	1.025180000
C	-2.590441000	1.046259000	1.695671000
C	-3.924864000	-1.558086000	0.321047000

H	5.082292000	-0.731484000	-0.339089000
H	3.928286000	0.466479000	0.279080000
H	4.091895000	0.041558000	-2.316741000
H	3.271097000	-1.475903000	-2.039283000
H	4.560249000	-1.590832000	2.423843000
H	3.397749000	-0.267595000	2.358959000
H	3.809473000	-2.474274000	0.421304000
H	2.387176000	-1.623597000	0.398674000
H	3.105936000	-2.371716000	4.009885000
H	2.394792000	-3.203483000	2.626747000
H	3.140238000	1.996210000	-1.408679000
H	2.146211000	2.040469000	-2.862597000
H	1.792854000	-0.657200000	-3.671199000
H	0.534822000	0.479997000	-3.193021000
H	1.406806000	-0.717067000	3.957271000
H	0.804367000	-2.232007000	4.109639000
H	0.846963000	-2.392738000	-2.078534000
H	-0.259534000	-1.154525000	-1.411291000
H	1.179550000	2.138073000	0.077502000
H	0.058758000	2.042131000	-1.308472000
H	1.946745000	4.303622000	-0.937314000
H	0.689608000	4.232942000	-1.980284000
H	-0.328280000	-2.369291000	-4.138241000
H	-1.259100000	-1.097864000	-3.726736000
H	0.787816000	-0.742507000	1.521262000
H	0.008963000	-2.320525000	1.874013000
H	-1.371214000	-3.936377000	-2.907124000
H	-2.641168000	-2.942991000	-3.620186000
H	0.583757000	4.377343000	1.008357000
H	0.361720000	5.703500000	-0.129403000
H	-1.623797000	-2.752509000	-0.667591000
H	-2.942966000	-3.784328000	-1.233482000
H	-0.708215000	0.418752000	3.124016000
H	-1.534696000	-1.083988000	3.530519000
H	-1.773081000	4.175790000	-0.996978000
H	-1.829578000	5.464623000	0.202389000
H	-0.672832000	1.975199000	1.244571000
H	-1.767301000	1.825649000	-0.153778000
H	-3.062193000	-0.816475000	-1.459284000
H	-4.273165000	-1.900931000	-1.704378000
H	-2.336237000	-2.369503000	1.540816000
H	-3.586243000	-1.462472000	2.366886000
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H	-3.080096000	3.682977000	0.909732000
H	-2.722783000	1.342198000	2.751918000
H	-3.599872000	1.017160000	1.261243000
H	-4.538042000	-2.450277000	0.524030000
H	-4.623943000	-0.711002000	0.261242000

$\text{H}_2\mathbf{5}^{5+}$

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N	-1.115101000	-1.414824000	2.413005000
N	-2.819610000	0.000659000	0.002345000
N	1.116876000	-1.385110000	-2.429707000
N	-1.121000000	-1.385296000	-2.428168000
N	1.117278000	2.797869000	0.016005000
N	-1.119921000	2.797018000	0.018375000
C	3.276748000	-0.521434000	1.372898000
H	3.253795000	0.328777000	2.067477000
H	4.330647000	-0.817143000	1.256437000
C	2.485317000	-1.713973000	1.937047000
H	2.434003000	-2.556371000	1.230990000
H	3.066979000	-2.090145000	2.795728000
C	0.003315000	-1.708600000	1.766683000
H	0.002788000	-2.190257000	0.786429000
C	-0.773806000	-0.978895000	3.810397000
H	-1.195544000	-1.703292000	4.523473000
H	-1.205699000	0.006936000	4.030306000
C	0.782463000	-0.979159000	3.809669000
H	1.214915000	0.006342000	4.029924000
H	1.204558000	-1.704506000	4.521605000
C	-2.478397000	-1.717015000	1.940518000
H	-3.057633000	-2.094907000	2.800066000
H	-2.426594000	-2.558913000	1.233917000
C	-3.273073000	-0.525441000	1.378649000
H	-4.326877000	-0.822344000	1.264492000
H	-3.249564000	0.324467000	2.073573000
C	3.275518000	-0.926718000	-1.144568000
H	3.256774000	-1.952431000	-0.752706000
H	4.328074000	-0.675325000	-1.346164000
C	2.479727000	-0.823681000	-2.457324000
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C	-0.780326000	-2.813628000	-2.749488000
H	-1.203085000	-3.068699000	-3.733001000
H	-1.211611000	-3.496772000	-2.005128000
C	0.776002000	-2.813519000	-2.750581000
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H	1.197468000	-3.068472000	-3.734674000
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H	-3.065007000	-1.382164000	-3.207251000
H	-2.432493000	0.206986000	-2.833498000
C	-3.277362000	-0.928480000	-1.139255000
H	-4.330466000	-0.677619000	-1.338656000
H	-3.257185000	-1.954409000	-0.748096000
C	3.275102000	1.456621000	-0.236816000

H	3.252556000	1.631449000	-1.320716000
H	4.328759000	1.505164000	0.078047000
C	2.481294000	2.540460000	0.512846000
H	2.430716000	2.352370000	1.595865000
H	3.060723000	3.473393000	0.407687000
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C	-0.780887000	3.788193000	-1.059537000
H	-1.202524000	4.768046000	-0.788880000
H	-1.213898000	3.484940000	-2.022527000
C	0.775296000	3.788788000	-1.061188000
H	1.206532000	3.486023000	-2.025124000
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C	-3.277527000	1.454126000	-0.229536000
H	-4.330251000	1.501516000	0.088667000
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C	-0.866610000	-1.123036000	3.771564000
O	-2.012928000	-1.123816000	2.918496000
C	-3.254129000	-1.065023000	3.642035000
C	-4.375145000	-1.285899000	2.647678000
N	-4.363668000	-0.227665000	1.557315000
C	-5.330364000	-0.488895000	0.421785000
C	-5.228858000	0.551921000	-0.688880000
C	5.140469000	0.921997000	0.723513000
C	4.562281000	2.332642000	0.621700000
N	4.152816000	2.716890000	-0.785451000
C	3.582290000	4.120046000	-0.993695000
C	2.377111000	4.437599000	-0.133584000
O	1.327333000	3.470786000	-0.359761000
C	0.201090000	3.667058000	0.514281000
C	-1.114991000	3.953076000	-0.196502000
N	-1.696759000	2.780041000	-0.962955000
C	-3.173099000	2.971610000	-1.261314000
C	-3.777801000	1.865699000	-2.120295000
C	5.013236000	-1.452392000	0.386917000
C	4.281862000	-2.723519000	-0.039990000
N	3.843829000	-2.710136000	-1.491743000

C	3.080964000	-3.934872000	-1.998409000
C	1.766020000	-4.201020000	-1.296893000
O	0.846475000	-3.106747000	-1.497439000
C	-0.450159000	-3.377141000	-0.930132000
C	-1.565062000	-2.851863000	-1.821032000
N	-1.488094000	-1.363590000	-2.064300000
C	-2.544194000	-0.834324000	-3.025673000
C	-3.908497000	-0.556892000	-2.403758000
N	-3.942252000	0.560608000	-1.432148000
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H	-3.155838000	1.733379000	-3.018611000
H	-3.277079000	3.936455000	-1.778296000
H	-3.673336000	3.066165000	-0.287772000
H	-1.856376000	4.231377000	0.566636000
H	-1.027419000	4.795307000	-0.896980000
H	0.376800000	4.519487000	1.190385000
H	0.089036000	2.768321000	1.146607000
H	2.052620000	5.454550000	-0.416841000
H	2.642390000	4.468547000	0.937600000
H	4.386681000	4.836658000	-0.773393000
H	3.346475000	4.186668000	-2.065184000
H	3.681696000	2.477806000	1.259275000
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H	5.962119000	0.816319000	-0.002446000
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H	-0.914817000	-1.949736000	4.503382000
H	-0.802915000	-0.181204000	4.351893000
H	0.272739000	-2.240233000	2.311532000
H	1.249158000	-1.443669000	3.580365000
H	1.574958000	-1.237280000	0.431769000
H	1.659269000	0.523990000	0.307997000
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H	2.933021000	-3.771620000	-3.075436000
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[F₂C₆H₂]⁵⁺

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N	3.502017000	3.161808000	-0.148199000
N	-1.582530000	-1.455822000	-2.217269000
N	1.986190000	-2.053000000	-1.703562000
N	-3.186589000	-0.980160000	2.048824000
N	0.972491000	-1.378330000	2.485615000
C	-3.641608000	2.252525000	-0.526785000
C	-2.563022000	3.115384000	-1.181181000
C	-0.193371000	4.068660000	-1.079694000
C	1.168381000	4.126055000	-0.370201000
C	2.080271000	2.909114000	-0.604918000
C	4.479304000	1.987094000	-0.298620000
C	4.369479000	0.889592000	0.768162000
C	-3.519442000	0.211877000	-1.864674000
C	-3.076231000	-1.243254000	-2.051325000
C	-1.241774000	-2.871828000	-2.670456000
C	0.169156000	-3.055235000	-3.239867000
C	1.354205000	-3.301000000	-2.300487000
C	3.293163000	-2.354865000	-0.999140000
C	4.087223000	-1.132062000	-0.544660000
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C	-4.258382000	0.068535000	1.825638000
C	-2.705402000	-1.201031000	3.479618000
C	-1.328913000	-1.873620000	3.489823000
C	-0.161306000	-0.873730000	3.350677000

C	2.270846000	-0.630656000	2.732198000
C	3.407357000	-1.047227000	1.797300000
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H	-1.259253000	-0.812466000	-2.954208000
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H	2.183262000	-1.395583000	-2.472189000
H	1.298740000	-1.589001000	-1.036551000
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H	-3.545932000	-1.884397000	1.703750000
H	1.136975000	-2.373803000	2.701719000
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H	3.052734000	-3.049168000	-0.183207000
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H	-1.232855000	-2.422349000	4.438425000
H	0.257009000	-0.634254000	4.337858000
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H	2.038166000	0.439354000	2.645236000
H	2.547279000	-0.831098000	3.777026000
H	3.320281000	-2.122420000	1.584746000
H	4.354010000	-0.958442000	2.362710000



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N	3.430410000	-0.961437000	3.434245000
C	-1.831304000	-3.115466000	-1.924385000
H	-2.549413000	-3.708896000	-2.506487000
H	-1.618042000	-3.682181000	-1.007143000
N	1.940227000	-2.560075000	-2.806630000
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H	-0.348201000	4.205363000	-0.148862000
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C	3.302346000	-1.105541000	-1.185817000
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C	0.697289000	-2.627429000	-1.939799000
H	0.641404000	-1.676423000	-1.390525000
H	0.877021000	-3.442314000	-1.223537000
C	3.264893000	-2.340057000	-2.063428000
H	3.438532000	-3.252325000	-1.478262000
H	4.037503000	-2.296885000	-2.847344000
N	-2.380777000	2.409179000	-0.437488000
N	-3.963235000	-0.051235000	0.611571000
C	3.611619000	-1.237925000	0.175444000
H	3.793111000	-2.239989000	0.576590000
C	3.179825000	0.184179000	-1.730343000
H	3.033297000	0.312914000	-2.807518000
C	3.645444000	1.166593000	0.429671000
H	3.860908000	2.045613000	1.045141000
C	3.338941000	1.326667000	-0.934227000
C	-3.861894000	2.131669000	-0.648403000
H	-3.952727000	1.630250000	-1.621687000
H	-4.369183000	3.103652000	-0.730348000
C	-3.829800000	-2.191063000	-0.718857000
H	-3.504764000	-2.771166000	0.155873000
H	-4.442154000	-2.857625000	-1.343109000
C	3.327793000	2.694325000	-1.584924000
H	4.196088000	3.296152000	-1.276523000
H	3.352038000	2.613958000	-2.679515000
C	4.313958000	-0.229679000	2.413859000
H	5.267524000	-0.781878000	2.421586000
H	4.507223000	0.759286000	2.849456000
C	-0.564089000	-2.899965000	-2.767692000
H	-0.432660000	-3.831108000	-3.343713000

H	-0.731092000	-2.107420000	-3.517082000
C	-4.478105000	1.328475000	0.493573000
H	-4.302705000	1.861765000	1.441791000
H	-5.576465000	1.357522000	0.352944000
C	-0.397320000	-0.201790000	3.325756000
H	-0.650555000	-0.492432000	4.355912000
H	-0.365230000	0.896218000	3.290825000
C	0.747612000	2.928947000	-1.549346000
H	0.708132000	1.986911000	-0.983836000
H	0.750961000	2.694191000	-2.623561000
C	0.939535000	-0.815977000	2.879824000
H	0.864984000	-1.916849000	2.925532000
H	1.143867000	-0.532702000	1.836215000
C	-1.807152000	3.323902000	-1.502486000
H	-2.504778000	4.168086000	-1.587756000
H	-1.842728000	2.777254000	-2.455063000
C	-4.644073000	-0.960884000	-0.333643000
H	-4.902857000	-0.400032000	-1.245687000
H	-5.612929000	-1.328798000	0.058367000
C	-2.883846000	-0.077394000	2.888401000
H	-2.781985000	1.016741000	2.905132000
H	-3.054149000	-0.406620000	3.923555000
C	-4.037184000	-0.543954000	2.002316000
H	-4.060636000	-1.645429000	1.994711000
H	-4.975267000	-0.244732000	2.509812000
C	2.078548000	-0.357534000	3.801316000
H	2.215456000	0.732532000	3.796347000
H	1.886569000	-0.663095000	4.840318000
F	-1.030450000	-0.004929000	-0.132356000
H	2.137885000	3.841626000	-0.263206000
H	2.193400000	4.436576000	-1.790478000
H	-1.607924000	-1.659322000	2.475387000
H	-1.357792000	-0.361896000	1.407828000
H	-2.861924000	-1.363377000	-2.362572000
H	1.824480000	-1.830241000	-3.527558000
H	3.307302000	-1.948261000	3.155893000
H	2.037754000	-3.443742000	-3.339109000
H	3.994322000	-1.007464000	4.302422000
H	-2.289798000	2.887373000	0.471256000
H	-1.970250000	-1.171792000	-0.947478000
H	-1.856638000	1.480573000	-0.355688000



C	-0.659928000	3.608626000	-0.454118000
C	0.773402000	3.624801000	0.074173000
C	-2.969734000	2.508642000	-0.393947000
N	1.657782000	2.517742000	-0.472918000
N	-1.557585000	2.563932000	0.187562000

C	3.075365000	2.497773000	0.097833000
C	3.874347000	1.310600000	-0.431282000
C	-3.816379000	1.424711000	0.267107000
C	-3.866289000	-0.425595000	-1.325042000
C	2.992463000	-1.190975000	-2.232202000
N	-1.642283000	-1.107363000	-2.305802000
N	-3.363057000	0.029159000	0.002800000
N	3.359437000	-0.022608000	-0.006393000
C	0.679463000	-1.767630000	-3.165855000
C	-3.059868000	-1.557421000	-1.955903000
C	3.823660000	-1.071904000	-0.957959000
N	1.573358000	-1.678067000	-1.940813000
C	-0.756091000	-2.202251000	-2.874697000
C	3.838882000	-0.335841000	1.370166000
C	-3.863421000	-0.879536000	1.073918000
C	-3.032025000	-0.874030000	2.353325000
N	1.595181000	-0.868687000	2.411215000
N	-1.629208000	-1.430730000	2.117653000
C	3.006217000	-1.374632000	2.115924000
C	-0.731063000	-1.403630000	3.342699000
C	0.696424000	-1.886718000	3.091972000
H	-0.707191000	3.463947000	-1.543482000
H	-1.111137000	4.590966000	-0.246745000
H	1.234795000	4.580255000	-0.218786000
H	0.819449000	3.575144000	1.171918000
H	-3.429590000	3.494796000	-0.233164000
H	-2.856640000	2.368652000	-1.477822000
H	1.738552000	2.646569000	-1.494148000
H	1.230705000	1.576085000	-0.310022000
H	-1.135591000	1.606243000	0.122331000
H	-1.646716000	2.792258000	1.190471000
H	3.561229000	3.440968000	-0.191700000
H	2.973210000	2.498814000	1.191754000
H	3.896593000	1.352485000	-1.531981000
H	4.925215000	1.465434000	-0.119644000
H	-4.859877000	1.587931000	-0.064734000
H	-3.836837000	1.596474000	1.355116000
H	-3.884045000	0.432875000	-2.015506000
H	-4.917339000	-0.769211000	-1.272851000
H	2.892420000	-0.240977000	-2.775067000
H	3.454829000	-1.916938000	-2.916990000
H	-1.723339000	-0.360684000	-3.014275000
H	-1.217667000	-0.679264000	-1.449483000
H	0.729281000	-0.799454000	-3.685517000
H	1.131288000	-2.511255000	-3.839913000
H	-3.539523000	-1.891756000	-2.887448000
H	-2.958390000	-2.434447000	-1.301820000
H	4.872051000	-0.907663000	-1.273369000
H	3.834153000	-2.045471000	-0.442518000
H	1.153928000	-1.055121000	-1.209077000
H	1.651117000	-2.622842000	-1.531818000
H	-1.213387000	-2.525814000	-3.822203000

H	-0.807233000	-3.061389000	-2.189976000
H	3.867657000	0.594338000	1.959750000
H	4.883083000	-0.703757000	1.368740000
H	-4.903885000	-0.639108000	1.366181000
H	-3.910976000	-1.906931000	0.679056000
H	-2.902893000	0.129563000	2.781412000
H	-3.512036000	-1.501525000	3.118497000
H	1.169961000	-0.529134000	1.515152000
H	1.685753000	-0.052802000	3.037361000
H	-1.199693000	-0.907193000	1.317625000
H	-1.734554000	-2.413742000	1.820170000
H	2.892269000	-2.316836000	1.562358000
H	3.478009000	-1.612733000	3.080515000
H	-0.765972000	-0.386104000	3.758968000
H	-1.189420000	-2.066895000	4.092011000
H	0.729749000	-2.810879000	2.496421000
H	1.154451000	-2.121250000	4.064928000
F	0.001806000	-0.006244000	0.008837000

[F₅C₂H₅]⁵⁺

F	0.000073000	0.001636000	0.001410000
N	-2.618119000	0.002980000	0.004619000
H	-1.537190000	0.001983000	0.003252000
N	-1.116679000	-2.129294000	-2.026231000
N	1.106118000	-2.129677000	-2.030222000
N	2.618570000	-0.000015000	-0.003721000
H	1.537934000	0.000847000	-0.000474000
N	-1.110944000	2.822805000	-0.828769000
N	1.111467000	2.821837000	-0.831232000
N	-1.106141000	-0.693838000	2.858118000
N	1.116186000	-0.695243000	2.855107000
C	-3.117349000	-0.790158000	-1.202166000
H	-3.002612000	-0.146009000	-2.083093000
H	-4.197277000	-0.943169000	-1.055166000
C	-2.470020000	-2.161336000	-1.471369000
H	-2.466202000	-2.806826000	-0.581606000
H	-3.123335000	-2.670757000	-2.197475000
C	-0.004044000	-2.248212000	-1.325040000
H	-0.002160000	-2.449853000	-0.257598000
C	0.769475000	-1.977911000	-3.475157000
H	1.187276000	-2.823788000	-4.039405000
H	1.196591000	-1.050728000	-3.881811000
C	-0.785148000	-1.975182000	-3.472078000
H	-1.210629000	-1.045322000	-3.874430000
H	-1.208119000	-2.817991000	-4.036998000
C	2.461508000	-2.162795000	-1.480493000
H	3.111423000	-2.672972000	-2.209075000
H	2.460326000	-2.808058000	-0.590554000
C	3.111521000	-0.792433000	-1.213457000

H	4.191987000	-0.946404000	-1.071671000
H	2.992918000	-0.147354000	-2.093216000
C	-3.113519000	1.445837000	-0.077432000
H	-2.994837000	1.886477000	0.920569000
H	-4.194061000	1.398245000	-0.280669000
C	-2.465893000	2.362470000	-1.131727000
H	-2.465001000	1.914225000	-2.135389000
H	-3.116764000	3.247874000	-1.209019000
C	-0.000503000	2.274758000	-1.286876000
H	-0.001570000	1.454988000	-1.999637000
C	0.778961000	3.993220000	0.029613000
H	1.198875000	4.906284000	-0.415807000
H	1.206961000	3.874852000	1.034774000
C	-0.775507000	3.993869000	0.031333000
H	-1.201390000	3.875567000	1.037364000
H	-1.195828000	4.907294000	-0.413070000
C	2.465231000	2.360506000	-1.138497000
H	3.116670000	3.245394000	-1.216881000
H	2.460795000	1.913222000	-2.142552000
C	3.115691000	1.442369000	-0.087167000
H	3.001902000	1.882676000	0.911626000
H	4.195266000	1.393232000	-0.295018000
C	-3.113778000	-0.646096000	1.296003000
H	-3.001116000	-1.731081000	1.176639000
H	-4.193189000	-0.440796000	1.359383000
C	-2.460107000	-0.195964000	2.615505000
H	-2.454490000	0.897187000	2.730865000
H	-3.109813000	-0.570100000	3.422664000
C	0.005119000	-0.025516000	2.610140000
H	0.005452000	1.001470000	2.256114000
C	0.782245000	-2.025698000	3.440331000
H	1.205187000	-2.097490000	4.452399000
H	1.206024000	-2.838266000	2.833926000
C	-0.772391000	-2.023537000	3.445166000
H	-1.202313000	-2.836803000	2.844124000
H	-1.189262000	-2.090702000	4.460156000
C	2.470130000	-0.199692000	2.607308000
H	3.122243000	-0.574554000	3.412164000
H	2.466590000	0.893546000	2.722224000
C	3.118088000	-0.650879000	1.285280000
H	3.002517000	-1.735693000	1.166189000
H	4.198103000	-0.447967000	1.344483000

Cartesian coordinate representation of the optimized molecular structures of H_61^{6+} , H_62^{6+} , H_63^{6+} , H_64^{6+} , H_25^{5+} , H_6222^{6+} , $[F\text{C}H_61]^{5+}$, $[F\text{C}H_62]^{5+}$, $[F\text{C}H_63]^{5+}$, $[F\text{C}H_64]^{5+}$ and $[F\text{C}H_25]^{4+}$ at B3P86/TZVP level of theory:

H_61^{6+}			
N	-3.142773000	1.683522000	0.362087000
C	-3.224386000	1.537849000	1.828628000
C	-3.080636000	0.077238000	2.275975000
N	-2.755803000	-0.044017000	3.737543000
C	-2.614503000	-1.454221000	4.290872000
C	-1.610337000	-2.322118000	3.555244000
O	-0.293902000	-1.780661000	3.535883000
C	4.157158000	-0.446425000	-0.585742000
C	3.562601000	0.913093000	-0.974608000
N	4.612758000	1.962284000	-1.212990000
C	4.108960000	3.304746000	-1.732585000
C	3.436912000	4.194586000	-0.713684000
O	2.105593000	3.765655000	-0.414662000
C	1.489055000	4.514255000	0.627745000
C	0.338529000	5.398024000	0.188345000
N	-0.877603000	4.666430000	-0.371222000
C	-1.396920000	3.506443000	0.433013000
C	-2.795663000	3.068173000	-0.019416000
N	3.113110000	-1.482775000	-0.432891000
C	3.564762000	-2.603722000	0.424519000
C	3.830646000	-2.312271000	1.893725000
N	2.626433000	-1.918498000	2.731020000
C	1.807890000	-3.032188000	3.342453000
C	0.714930000	-2.496265000	4.253134000
C	-4.432719000	1.321101000	-0.273603000
C	-4.369306000	0.967434000	-1.758050000
N	-3.966304000	-0.459350000	-2.035626000
C	-3.670528000	-0.776394000	-3.483953000
C	-3.109454000	-2.171432000	-3.634282000
O	-1.888984000	-2.259345000	-2.886190000
C	-1.409001000	-3.583332000	-2.665960000
C	-0.177330000	-3.937622000	-3.474085000
N	1.010661000	-3.015525000	-3.242255000
C	1.473533000	-2.831197000	-1.823198000
C	2.762835000	-2.002578000	-1.771788000
H	-2.839903000	3.120571000	-1.110200000
H	-3.541539000	3.784505000	0.355380000
H	-0.679467000	2.695279000	0.313672000
H	-1.389239000	3.839125000	1.470658000

H	-0.657657000	4.356695000	-1.320523000
H	-1.613567000	5.374462000	-0.477450000
H	0.634028000	6.108128000	-0.585466000
H	-0.015468000	5.968846000	1.049128000
H	2.203183000	5.189971000	1.108890000
H	1.163799000	3.813542000	1.401822000
H	4.033406000	4.252460000	0.205707000
H	3.430467000	5.199160000	-1.150775000
H	4.996058000	3.823825000	-2.101553000
H	3.464983000	3.090818000	-2.585268000
H	5.292156000	1.615499000	-1.899750000
H	5.159799000	2.126444000	-0.361456000
H	2.900401000	1.300441000	-0.202942000
H	2.996889000	0.856836000	-1.904060000
H	4.916023000	-0.755396000	-1.319805000
H	4.683744000	-0.338183000	0.363221000
H	2.819034000	-3.397249000	0.352898000
H	4.501440000	-3.041904000	0.049503000
H	4.565066000	-1.519819000	2.033542000
H	4.253798000	-3.207518000	2.351814000
H	2.971054000	-1.344183000	3.505378000
H	2.010361000	-1.320385000	2.176330000
H	1.406232000	-3.634161000	2.528607000
H	2.496230000	-3.646485000	3.926318000
H	1.138692000	-1.833313000	5.014667000
H	0.293793000	-3.353086000	4.785649000
H	-1.927137000	-2.493383000	2.522850000
H	-1.637103000	-3.295874000	4.053011000
H	-2.350035000	-1.329131000	5.342129000
H	-3.601679000	-1.917797000	4.244273000
H	-3.479950000	0.422307000	4.296327000
H	-1.885763000	0.454391000	3.939942000
H	-3.990980000	-0.501758000	2.119332000
H	-2.262452000	-0.392340000	1.732758000
H	-4.148963000	1.974005000	2.232430000
H	-2.398904000	2.103311000	2.267245000
H	-5.159129000	2.139227000	-0.177001000
H	-4.875113000	0.486341000	0.275396000
H	-3.672730000	1.596599000	-2.310339000
H	-5.354013000	1.101683000	-2.207836000
H	-4.714100000	-1.081966000	-1.715066000
H	-3.128347000	-0.700431000	-1.500884000
H	-4.597622000	-0.676478000	-4.050153000
H	-2.965932000	-0.022028000	-3.832973000
H	-3.822894000	-2.924027000	-3.279717000
H	-2.945106000	-2.350771000	-4.701144000
H	-1.214526000	-3.692745000	-1.596029000
H	-2.164728000	-4.332039000	-2.922109000
H	0.146361000	-4.949450000	-3.222853000
H	-0.365173000	-3.902925000	-4.548507000
H	0.776806000	-2.105885000	-3.647312000
H	1.781495000	-3.384693000	-3.810859000

H	0.669685000	-2.328000000	-1.288102000
H	1.601047000	-3.833512000	-1.414829000
H	3.592659000	-2.594007000	-2.187242000
H	2.633323000	-1.142302000	-2.432773000

H₆2⁶⁺

N	-2.834010000	-0.591046000	0.665389000
C	-3.387347000	-1.965967000	0.600314000
C	-2.449439000	-3.056569000	0.073150000
N	-2.437780000	-3.227161000	-1.436037000
C	-1.185471000	-3.828344000	-2.047850000
C	0.010261000	-2.880856000	-1.928768000
C	1.214319000	-3.341813000	-2.752886000
N	2.458183000	-2.536445000	-2.424433000
C	2.463107000	-1.078414000	-2.848953000
C	3.391493000	-0.165237000	-2.042052000
C	-1.710438000	-0.434650000	1.599078000
C	-1.886687000	-0.894157000	3.067762000
N	-0.787593000	-0.362680000	3.975501000
C	0.644804000	-0.781761000	3.669166000
C	1.643920000	0.321277000	4.026448000
C	3.123284000	0.000208000	3.812360000
N	3.618002000	-0.096874000	2.368974000
C	3.574382000	1.165058000	1.539182000
C	3.907065000	0.973069000	0.057020000
C	-3.913931000	0.404801000	0.864186000
C	-3.584880000	1.852722000	0.490097000
N	-3.625433000	2.153089000	-0.990055000
C	-3.133038000	3.530286000	-1.435281000
C	-1.654005000	3.850732000	-1.218290000
C	-0.654071000	3.107221000	-2.107081000
N	0.777075000	3.554397000	-1.838207000
C	1.879452000	2.516799000	-1.987467000
C	1.706117000	1.330275000	-1.006396000
N	2.832228000	0.410450000	-0.794943000
H	-4.290692000	-1.936100000	-0.014071000
H	-3.740539000	-2.311608000	1.579892000
H	-2.757900000	-4.021921000	0.475529000
H	-1.418610000	-2.892660000	0.378027000
H	-2.632634000	-2.333908000	-1.892381000
H	-3.223168000	-3.837734000	-1.695588000
H	-1.432608000	-4.039120000	-3.090362000
H	-1.013317000	-4.783042000	-1.548755000
H	0.311896000	-2.804851000	-0.879430000
H	-0.297889000	-1.883935000	-2.259217000
H	1.047122000	-3.246398000	-3.826712000
H	1.469477000	-4.383656000	-2.548178000
H	3.250402000	-3.005625000	-2.881830000
H	2.645749000	-2.611325000	-1.422661000

H	1.429930000	-0.740639000	-2.819696000
H	2.776386000	-1.077471000	-3.893398000
H	3.733587000	0.613883000	-2.734618000
H	4.302316000	-0.710906000	-1.783225000
H	-1.441959000	0.625770000	1.604435000
H	-0.851288000	-0.956098000	1.170427000
H	-1.869417000	-1.978465000	3.176624000
H	-2.820415000	-0.535328000	3.503807000
H	-1.014125000	-0.660300000	4.933792000
H	-0.845976000	0.659615000	4.009792000
H	0.668829000	-1.029037000	2.609094000
H	0.830424000	-1.695344000	4.235593000
H	1.575599000	0.536272000	5.098656000
H	1.378896000	1.257270000	3.524552000
H	3.403738000	-0.943835000	4.283871000
H	3.726005000	0.781532000	4.277711000
H	3.134828000	-0.847866000	1.874894000
H	4.597252000	-0.401079000	2.434831000
H	4.308478000	1.841937000	1.979672000
H	2.592828000	1.609098000	1.694842000
H	4.782633000	0.325535000	-0.033275000
H	4.254796000	1.950424000	-0.300825000
H	-4.265400000	0.437409000	1.903115000
H	-4.786507000	0.075431000	0.294849000
H	-2.604812000	2.164391000	0.846581000
H	-4.321816000	2.511841000	0.952232000
H	-4.603743000	2.098138000	-1.299416000
H	-3.138552000	1.416828000	-1.502129000
H	-3.735993000	4.251061000	-0.881026000
H	-3.414878000	3.618188000	-2.486506000
H	-1.388408000	3.736618000	-0.162490000
H	-1.587247000	4.925506000	-1.420677000
H	-0.842292000	3.285668000	-3.166658000
H	-0.673719000	2.032157000	-1.935172000
H	0.835925000	3.973719000	-0.905241000
H	0.999672000	4.329480000	-2.476932000
H	2.811638000	3.058775000	-1.819794000
H	1.863239000	2.207338000	-3.032353000
H	0.849106000	0.733880000	-1.328408000
H	1.435071000	1.736298000	-0.027532000

H₆3⁶⁺

N	-2.325663000	3.687133000	-0.575176000
H	-2.738682000	4.628770000	-0.614632000
H	-2.045621000	3.483254000	-1.537028000
N	-1.981486000	-2.001419000	3.446956000
H	-1.928532000	-2.896139000	2.951642000
H	-2.242443000	-2.255031000	4.409926000
N	-2.475834000	-2.118502000	-3.154725000
H	-2.441919000	-1.274026000	-3.732725000

H	-2.830756000	-2.849105000	-3.787256000
N	2.272031000	3.757531000	-0.468114000
H	3.079145000	4.081323000	-1.015805000
H	2.476726000	4.059227000	0.491217000
N	2.526106000	-1.619083000	2.539427000
H	1.828919000	-1.504837000	1.803538000
H	2.908095000	-2.564767000	2.435050000
N	2.045605000	-1.520332000	-2.875748000
H	1.399331000	-0.965755000	-2.314504000
H	2.245820000	-0.972386000	-3.718841000
N	3.320621000	0.059708000	-0.182566000
C	-3.158374000	1.273798000	-0.020071000
C	-3.257562000	0.401834000	-1.108266000
H	-3.489307000	0.805805000	-2.090372000
C	-3.202424000	-0.986420000	-0.932689000
C	-3.083210000	-1.494063000	0.364262000
H	-3.165630000	-2.567546000	0.509315000
C	-2.998224000	-0.650087000	1.475250000
C	-3.023766000	0.728730000	1.261521000
H	-3.046258000	1.392392000	2.120280000
C	-3.468557000	2.751458000	-0.163307000
H	-4.246349000	2.911377000	-0.912663000
H	-3.843102000	3.154703000	0.777927000
C	-3.137542000	-1.170603000	2.892854000
H	-3.269355000	-0.346680000	3.593534000
H	-4.018369000	-1.811696000	2.980769000
C	-3.530104000	-1.949076000	-2.057657000
H	-3.707499000	-2.950212000	-1.666097000
H	-4.438901000	-1.642927000	-2.581442000
C	-1.135079000	3.715609000	0.349757000
H	-0.751497000	2.696011000	0.373419000
H	-1.549775000	3.937896000	1.333637000
C	-0.070336000	4.775437000	0.029425000
H	-0.567233000	5.694889000	-0.300775000
H	0.369895000	5.076887000	0.985898000
C	1.052134000	4.530460000	-0.983011000
H	0.741348000	4.026103000	-1.898673000
H	1.448412000	5.503933000	-1.277413000
C	-0.640990000	-1.323434000	3.453016000
H	-0.751394000	-0.437389000	4.080404000
H	-0.482565000	-0.992915000	2.423738000
C	0.494288000	-2.210110000	3.972184000
H	0.324061000	-2.446064000	5.027029000
H	0.522582000	-3.177582000	3.458613000
C	1.865940000	-1.532126000	3.909398000
H	1.814121000	-0.474862000	4.171299000
H	2.553990000	-2.007220000	4.609224000
C	-1.096975000	-2.485417000	-2.684654000
H	-1.194204000	-3.441803000	-2.168230000
H	-0.838672000	-1.725617000	-1.943191000
C	-0.067117000	-2.587683000	-3.814431000
H	-0.105566000	-1.716965000	-4.478972000

H	-0.301860000	-3.446606000	-4.450083000
C	1.364886000	-2.808259000	-3.315829000
H	1.409830000	-3.499013000	-2.473121000
H	1.982117000	-3.223801000	-4.113093000
C	2.193303000	2.255517000	-0.555598000
H	2.028277000	2.038209000	-1.611596000
H	1.311974000	1.947196000	0.005157000
C	3.434825000	1.530577000	-0.023035000
H	4.343004000	1.911767000	-0.509750000
H	3.545407000	1.760821000	1.038130000
C	3.638158000	-0.621529000	2.284030000
H	3.258219000	0.348687000	2.602758000
H	4.455278000	-0.886374000	2.957529000
C	4.153859000	-0.622801000	0.848451000
H	4.318306000	-1.655061000	0.528072000
H	5.157296000	-0.177579000	0.887213000
C	3.338075000	-1.663727000	-2.092859000
H	4.072640000	-2.074935000	-2.787011000
H	3.157478000	-2.413223000	-1.323076000
C	3.838676000	-0.333428000	-1.524488000
H	4.934500000	-0.389341000	-1.506694000
H	3.615753000	0.465019000	-2.238161000

H₆4⁶⁺

C	3.973039000	-0.550518000	-0.236158000
C	3.333624000	-0.508825000	-1.621829000
C	3.446062000	-1.354628000	2.164748000
N	3.311009000	-1.584725000	0.671462000
C	2.523830000	-2.201052000	3.041269000
N	2.014297000	0.177196000	-1.685515000
C	2.178287000	1.651062000	-1.782588000
C	1.168903000	-0.348581000	-2.783326000
N	1.182544000	-1.566987000	3.406270000
C	0.260151000	-1.489158000	-2.292042000
C	1.069568000	2.350059000	-0.981467000
N	1.049841000	3.859289000	-1.029828000
N	-0.796875000	-1.907895000	-3.288664000
C	0.221916000	-1.302986000	2.270994000
C	-1.858342000	-2.913210000	-2.815999000
C	0.211239000	4.577577000	0.031403000
C	-2.414965000	-2.780987000	-1.400688000
C	-1.032064000	-0.513488000	2.683024000
N	-1.949503000	-0.266595000	1.541444000
C	-1.317117000	4.442109000	-0.044721000
C	-1.672003000	2.070734000	0.897513000
N	-3.388213000	-1.660380000	-1.135403000
C	-2.922207000	-1.388181000	1.460847000
N	-2.004132000	3.539047000	0.982759000
C	-2.570365000	1.077161000	1.653874000

C	-3.910567000	-1.499107000	0.303000000
H	5.028150000	-0.819287000	-0.313437000
H	3.912941000	0.406957000	0.280687000
H	4.063740000	-0.039179000	-2.292206000
H	3.221732000	-1.528224000	-2.002739000
H	4.479175000	-1.599722000	2.422986000
H	3.327693000	-0.284900000	2.344269000
H	3.709674000	-2.504521000	0.447616000
H	2.325754000	-1.620361000	0.408297000
H	3.028007000	-2.370789000	3.996947000
H	2.311731000	-3.188244000	2.624715000
H	3.149774000	1.924631000	-1.365853000
H	2.192405000	1.984866000	-2.826995000
H	1.774377000	-0.671843000	-3.638417000
H	0.538907000	0.465391000	-3.153022000
H	1.361674000	-0.707482000	3.939177000
H	0.742022000	-2.199770000	4.089661000
H	0.824583000	-2.393941000	-2.060697000
H	-0.260584000	-1.158381000	-1.392671000
H	1.173514000	2.086850000	0.069742000
H	0.091030000	2.025051000	-1.330277000
H	2.005528000	4.224183000	-0.912823000
H	0.772047000	4.190550000	-1.962882000
H	-0.344880000	-2.350038000	-4.102532000
H	-1.254465000	-1.082634000	-3.688500000
H	0.766169000	-0.729395000	1.518585000
H	-0.031223000	-2.283195000	1.864489000
H	-1.384551000	-3.896565000	-2.865449000
H	-2.638198000	-2.909316000	-3.582587000
H	0.624068000	4.294020000	1.001237000
H	0.451119000	5.635245000	-0.106441000
H	-1.630034000	-2.708825000	-0.652095000
H	-2.957554000	-3.711275000	-1.209098000
H	-0.714721000	0.449752000	3.089350000
H	-1.553357000	-1.027616000	3.501138000
H	-1.675202000	4.128144000	-1.026825000
H	-1.743401000	5.432662000	0.134994000
H	-0.646704000	1.979018000	1.251392000
H	-1.695262000	1.827165000	-0.163064000
H	-3.005801000	-0.763965000	-1.433934000
H	-4.227933000	-1.806515000	-1.713027000
H	-2.349831000	-2.315679000	1.529983000
H	-3.583880000	-1.397859000	2.340241000
H	-1.822194000	3.900978000	1.927895000
H	-3.014206000	3.687187000	0.850073000
H	-2.722199000	1.376039000	2.697662000
H	-3.562152000	1.060261000	1.199667000
H	-4.522869000	-2.383620000	0.495586000
H	-4.601343000	-0.656344000	0.244388000

$\text{H}_2\mathbf{5}^{5+}$

N	-2.800607000	0.000332000	0.000259000
N	-1.110153000	-1.896938000	-2.007789000
N	1.108515000	-1.896887000	-2.008031000
N	2.800652000	-0.000692000	-0.000588000
N	-1.109083000	-0.791413000	2.646046000
N	1.109719000	-0.791731000	2.645820000
N	-1.108734000	2.688834000	-0.638892000
N	1.109686000	2.688477000	-0.639205000
C	-3.256368000	-0.816349000	-1.206267000
H	-3.237962000	-0.153825000	-2.070805000
H	-4.300586000	-1.078997000	-1.023627000
C	-2.463940000	-2.093424000	-1.483825000
H	-2.409786000	-2.748714000	-0.612510000
H	-3.035658000	-2.653235000	-2.230163000
C	-0.000762000	-2.047056000	-1.323085000
H	-0.000635000	-2.304016000	-0.269739000
C	0.772329000	-1.775464000	-3.457088000
H	1.189995000	-2.630662000	-3.991499000
H	1.199948000	-0.867900000	-3.882264000
C	-0.774320000	-1.775930000	-3.456957000
H	-1.202555000	-0.868848000	-3.882516000
H	-1.191598000	-2.631678000	-3.990803000
C	2.462357000	-2.094229000	-1.484492000
H	3.033473000	-2.654543000	-2.230913000
H	2.408006000	-2.749334000	-0.613056000
C	3.255611000	-0.817605000	-1.207275000
H	4.299763000	-1.080761000	-1.024989000
H	3.237237000	-0.155079000	-2.071814000
C	-3.256730000	-0.635507000	1.311131000
H	-3.240286000	-1.715379000	1.169580000
H	-4.300334000	-0.344023000	1.448074000
C	-2.462703000	-0.238499000	2.555344000
H	-2.407906000	0.843651000	2.686999000
H	-3.033876000	-0.604727000	3.413828000
C	0.000401000	-0.123418000	2.433692000
H	0.000525000	0.917204000	2.129041000
C	0.773450000	-2.107096000	3.265643000
H	1.191325000	-2.141749000	4.273400000
H	1.201033000	-2.929166000	2.692531000
C	-0.773054000	-2.106864000	3.265841000
H	-1.201040000	-2.928824000	2.692875000
H	-1.190674000	-2.141339000	4.273709000
C	2.463505000	-0.239320000	2.554615000
H	3.034827000	-0.605688000	3.412939000
H	2.409135000	0.842864000	2.686193000
C	3.256962000	-0.636688000	1.310150000
H	4.300721000	-0.345601000	1.446755000
H	3.240099000	-1.716559000	1.168638000
C	-3.255102000	1.454243000	-0.103303000

H	-3.236524000	1.870988000	0.903004000
H	-4.299474000	1.428214000	-0.421917000
C	-2.462777000	2.333472000	-1.070425000
H	-2.408977000	1.906530000	-2.073483000
H	-3.034397000	3.259846000	-1.181586000
C	0.000326000	2.170486000	-1.111576000
H	0.000092000	1.385882000	-1.859934000
C	0.774036000	3.881764000	0.191989000
H	1.191733000	4.772852000	-0.280196000
H	1.201740000	3.794748000	1.190393000
C	-0.772469000	3.882019000	0.192200000
H	-1.199926000	3.795173000	1.190724000
H	-1.190002000	4.773231000	-0.279898000
C	2.463496000	2.332671000	-1.071091000
H	3.035456000	3.258849000	-1.182152000
H	2.409370000	1.905952000	-2.074226000
C	3.255747000	1.453008000	-0.104299000
H	4.299977000	1.426559000	-0.423355000
H	3.237770000	1.869748000	0.902021000
H	-1.778888000	-0.001106000	0.001190000
H	1.778927000	-0.001694000	0.000677000



N	4.141933000	-0.202320000	0.504530000
C	3.145198000	-0.308758000	1.589878000
C	1.735897000	-0.319409000	1.004976000
N	0.607643000	-0.197129000	1.978295000
C	0.388374000	-1.343844000	2.917720000
C	-0.846404000	-1.147174000	3.764800000
O	-1.976387000	-1.122738000	2.915735000
C	-3.212925000	-1.065101000	3.615602000
C	-4.316675000	-1.278098000	2.612947000
N	-4.283176000	-0.232424000	1.529995000
C	-5.251665000	-0.484919000	0.411528000
C	-5.161487000	0.554771000	-0.688530000
C	5.077788000	0.924484000	0.717919000
C	4.493895000	2.323176000	0.614557000
N	4.088285000	2.695260000	-0.782115000
C	3.530874000	4.086932000	-0.991650000
C	2.332277000	4.398678000	-0.133324000
O	1.315102000	3.414106000	-0.328526000
C	0.200824000	3.583107000	0.539898000
C	-1.107045000	3.892074000	-0.158108000
N	-1.682349000	2.745462000	-0.941224000
C	-3.137911000	2.955491000	-1.258835000
C	-3.734136000	1.859178000	-2.119503000
C	4.953523000	-1.431308000	0.372834000
C	4.219415000	-2.687676000	-0.061862000
N	3.791771000	-2.658001000	-1.501822000

C	3.053388000	-3.874291000	-2.019435000
C	1.749318000	-4.156391000	-1.320560000
O	0.845939000	-3.061804000	-1.476748000
C	-0.436331000	-3.322739000	-0.911756000
C	-1.545983000	-2.811647000	-1.802703000
N	-1.467072000	-1.337864000	-2.050019000
C	-2.505359000	-0.819935000	-3.014331000
C	-3.863893000	-0.544182000	-2.400755000
N	-3.893804000	0.564529000	-1.438233000
F	-1.136405000	0.297292000	0.128598000
H	-4.692770000	2.235110000	-2.501519000
H	-3.112307000	1.732583000	-3.008193000
H	-3.222981000	3.913230000	-1.774483000
H	-3.650462000	3.055464000	-0.302059000
H	-1.842122000	4.155010000	0.604133000
H	-1.015870000	4.742590000	-0.834492000
H	0.379229000	4.402733000	1.241431000
H	0.084500000	2.669320000	1.132000000
H	1.986056000	5.394696000	-0.428832000
H	2.604822000	4.453201000	0.925814000
H	4.329792000	4.797486000	-0.774433000
H	3.293499000	4.155094000	-2.053812000
H	3.617803000	2.460324000	1.245693000
H	5.248382000	3.044320000	0.932277000
H	5.893262000	0.825777000	-0.002996000
H	5.552600000	0.864145000	1.706863000
H	-5.317947000	1.544588000	-0.251720000
H	-6.022451000	0.393905000	-1.352459000
H	-6.253914000	-0.476625000	0.841776000
H	-5.061208000	-1.497682000	0.058071000
H	-5.293783000	-1.232153000	3.094509000
H	-4.215296000	-2.245431000	2.122319000
H	-3.317520000	-0.106633000	4.139804000
H	-3.283055000	-1.859323000	4.366293000
H	-0.901856000	-1.981039000	4.473693000
H	-0.779004000	-0.224461000	4.357656000
H	0.292090000	-2.243754000	2.310020000
H	1.260294000	-1.444502000	3.563900000
H	1.545499000	-1.229044000	0.432447000
H	1.618428000	0.520626000	0.319205000
H	3.331112000	-1.200476000	2.195902000
H	3.250274000	0.535193000	2.278617000
H	5.448193000	-1.681880000	1.321567000
H	5.762351000	-1.229851000	-0.334209000
H	4.885520000	-3.544097000	0.052045000
H	3.329822000	-2.881986000	0.534575000
H	2.900274000	-3.702826000	-3.085617000
H	3.720480000	-4.730029000	-1.904383000
H	1.896795000	-4.381671000	-0.258508000
H	1.342803000	-5.061155000	-1.785278000
H	-0.501312000	-2.871607000	0.085492000
H	-0.597884000	-4.398080000	-0.794139000

H	-1.511746000	-3.300407000	-2.777004000
H	-2.509064000	-3.034918000	-1.345065000
H	-2.610078000	-1.560539000	-3.807895000
H	-2.081598000	0.072687000	-3.472774000
H	-4.232164000	-1.447264000	-1.910381000
H	-4.551190000	-0.372769000	-3.242235000
H	3.398204000	2.017822000	-1.110204000
H	4.901681000	2.602795000	-1.397632000
H	-1.540351000	1.820664000	-0.450132000
H	-1.168072000	2.675718000	-1.820207000
H	-3.327746000	-0.164197000	1.151686000
H	-4.497584000	0.674476000	1.951673000
H	0.731808000	0.647508000	2.539288000
H	-0.251795000	-0.034063000	1.351690000
H	-1.471846000	-0.772060000	-1.158777000
H	-0.551419000	-1.173142000	-2.469486000
H	3.217186000	-1.828254000	-1.660168000
H	4.625700000	-2.544384000	-2.086130000

[F₆H₂]⁵⁺

F	0.015146000	-1.106329000	-0.059297000
N	-3.409411000	0.769592000	-0.476405000
N	3.447435000	-0.282776000	0.504980000
N	-1.257795000	3.199753000	-0.359360000
N	3.462778000	3.151189000	-0.127103000
N	-1.567130000	-1.427553000	-2.205285000
N	1.972859000	-2.019049000	-1.703391000
N	-3.142238000	-0.995792000	2.019884000
N	0.972818000	-1.396887000	2.455585000
C	-3.617375000	2.236309000	-0.502291000
C	-2.548095000	3.103208000	-1.146674000
C	-0.207221000	4.054336000	-1.037590000
C	1.146916000	4.109474000	-0.332594000
C	2.052508000	2.900604000	-0.573781000
C	4.425311000	1.984894000	-0.287039000
C	4.312061000	0.889886000	0.771101000
C	-3.487299000	0.227216000	-1.849884000
C	-3.048206000	-1.218601000	-2.045424000
C	-1.231729000	-2.829964000	-2.658835000
C	0.169416000	-3.009746000	-3.230367000
C	1.348119000	-3.255895000	-2.297267000
C	3.277496000	-2.319429000	-1.023134000
C	4.057666000	-1.101939000	-0.559470000
C	-4.511443000	0.189104000	0.334415000
C	-4.206377000	0.044615000	1.812830000
C	-2.676407000	-1.231503000	3.438848000
C	-1.308464000	-1.900458000	3.447248000
C	-0.150914000	-0.902456000	3.315771000

C	2.256515000	-0.652626000	2.703086000
C	3.381381000	-1.055887000	1.762972000
H	-1.467405000	3.607982000	0.556100000
H	-0.916041000	2.251802000	-0.189412000
H	3.847818000	3.937861000	-0.663587000
H	3.484096000	3.465203000	0.848659000
H	-1.242739000	-0.786124000	-2.930535000
H	-1.032218000	-1.214408000	-1.318634000
H	2.155378000	-1.358930000	-2.460948000
H	1.297400000	-1.571334000	-1.032293000
H	-2.350354000	-0.742812000	1.417827000
H	-3.495276000	-1.888073000	1.664218000
H	1.138201000	-2.384810000	2.662838000
H	0.671050000	-1.323843000	1.443384000
H	-4.544756000	2.484110000	-1.039938000
H	-3.782723000	2.577570000	0.523502000
H	-2.932451000	4.120807000	-1.232975000
H	-2.270922000	2.779069000	-2.148960000
H	-0.632550000	5.057178000	-1.085493000
H	-0.119605000	3.689200000	-2.061521000
H	1.630089000	5.004966000	-0.737477000
H	1.018719000	4.308236000	0.736342000
H	2.120770000	2.679253000	-1.640332000
H	1.730927000	1.993608000	-0.057889000
H	4.309576000	1.633273000	-1.311186000
H	5.417159000	2.433252000	-0.212372000
H	3.994996000	1.342816000	1.715708000
H	5.342148000	0.551818000	0.955841000
H	-4.516352000	0.292308000	-2.229074000
H	-2.899851000	0.860289000	-2.518960000
H	-3.507948000	-1.587677000	-2.963317000
H	-3.376694000	-1.882098000	-1.246103000
H	-1.416580000	-3.492528000	-1.813093000
H	-1.954868000	-3.077482000	-3.436163000
H	0.104526000	-3.916389000	-3.840234000
H	0.400310000	-2.226897000	-3.963063000
H	2.137980000	-3.754223000	-2.859745000
H	1.078870000	-3.906619000	-1.464833000
H	3.055066000	-3.023206000	-0.221930000
H	3.897070000	-2.856775000	-1.743070000
H	4.248713000	-0.464962000	-1.426615000
H	5.044364000	-1.482426000	-0.254409000
H	-5.429411000	0.781662000	0.238868000
H	-4.773993000	-0.793512000	-0.064291000
H	-5.096718000	-0.273661000	2.357150000
H	-3.845871000	0.965698000	2.270795000
H	-2.673332000	-0.268246000	3.949679000
H	-3.429943000	-1.855117000	3.919045000
H	-1.269898000	-2.660297000	2.659097000
H	-1.211620000	-2.451926000	4.384115000
H	0.261821000	-0.668917000	4.297362000
H	-0.466828000	0.041285000	2.866975000

H	2.023577000	0.409434000	2.627699000
H	2.537217000	-0.859396000	3.736535000
H	3.289597000	-2.119444000	1.538938000
H	4.324831000	-0.975781000	2.317592000



N	-1.535773000	-0.377132000	2.479686000
N	2.083848000	3.368974000	-1.609827000
N	3.400730000	-0.569241000	3.494847000
C	-1.823988000	-3.267998000	-1.596655000
H	-2.539245000	-3.901030000	-2.121861000
H	-1.619676000	-3.748695000	-0.639169000
N	1.927372000	-2.823611000	-2.498224000
C	-0.397499000	3.699241000	-1.591610000
H	-0.308238000	4.543756000	-2.281233000
H	-0.339144000	4.132362000	-0.586895000
N	-2.543974000	-1.982062000	-1.300851000
C	3.271351000	-1.223828000	-1.043394000
C	3.753922000	-0.000747000	0.998941000
C	0.692848000	-2.809202000	-1.640105000
H	0.641087000	-1.822489000	-1.176931000
H	0.861107000	-3.556016000	-0.862554000
C	3.233660000	-2.540248000	-1.777543000
H	3.393911000	-3.376717000	-1.098685000
H	4.011235000	-2.585925000	-2.544114000
N	-2.353454000	2.328419000	-0.678422000
N	-3.928505000	0.015404000	0.614858000
C	3.580409000	-1.205261000	0.313034000
H	3.760136000	-2.149122000	0.819336000
C	3.147516000	-0.011503000	-1.722877000
H	2.998374000	-0.003539000	-2.798617000
C	3.613814000	1.194859000	0.299434000
H	3.826980000	2.130307000	0.808523000
C	3.307913000	1.202160000	-1.063430000
C	-3.821965000	2.036001000	-0.855091000
H	-3.916772000	1.434452000	-1.759241000
H	-4.323667000	2.986606000	-1.041622000
C	-3.791358000	-2.227799000	-0.490805000
H	-3.471984000	-2.713947000	0.431503000
H	-4.400125000	-2.947389000	-1.040308000
C	3.296966000	2.484212000	-1.855874000
H	4.166139000	3.103329000	-1.624476000
H	3.312267000	2.285095000	-2.926746000
C	4.280078000	0.035025000	2.413086000
H	5.225539000	-0.509724000	2.478288000
H	4.475356000	1.058569000	2.730679000
C	-0.559193000	-3.139056000	-2.444599000
H	-0.432475000	-4.108855000	-2.934930000

H	-0.712651000	-2.415888000	-3.252318000
C	-4.432569000	1.367780000	0.361548000
H	-4.245877000	1.992054000	1.239943000
H	-5.522976000	1.387078000	0.228771000
C	-0.400320000	0.153840000	3.296035000
H	-0.646269000	-0.013308000	4.346187000
H	-0.372184000	1.231946000	3.134441000
C	0.746076000	2.721997000	-1.835288000
H	0.702547000	1.851185000	-1.179211000
H	0.746773000	2.377819000	-2.870703000
C	0.929721000	-0.498917000	2.924084000
H	0.862323000	-1.578356000	3.100012000
H	1.128581000	-0.342989000	1.861497000
C	-1.790311000	3.117586000	-1.827273000
H	-2.484211000	3.940025000	-2.000686000
H	-1.825047000	2.477569000	-2.709361000
C	-4.600358000	-0.971514000	-0.235087000
H	-4.848838000	-0.507003000	-1.193089000
H	-5.565011000	-1.292054000	0.182356000
C	-2.865505000	0.215460000	2.865571000
H	-2.767257000	1.297051000	2.769267000
H	-3.034411000	-0.003295000	3.920987000
C	-4.009265000	-0.336968000	2.034664000
H	-4.029132000	-1.425517000	2.134925000
H	-4.943329000	0.007193000	2.499064000
C	2.060191000	0.070729000	3.776332000
H	2.193855000	1.143026000	3.631983000
H	1.864385000	-0.096596000	4.836754000
F	-1.029640000	-0.022897000	-0.127953000
H	2.128725000	3.749121000	-0.660787000
H	2.177673000	4.185690000	-2.226038000
H	-1.596899000	-1.385687000	2.631550000
H	-1.359887000	-0.230314000	1.435430000
H	-2.830305000	-1.571297000	-2.191754000
H	1.816462000	-2.168661000	-3.276534000
H	3.280267000	-1.573001000	3.334435000
H	2.023949000	-3.744542000	-2.943195000
H	3.954141000	-0.515109000	4.358699000
H	-2.259532000	2.893973000	0.167327000
H	-1.939284000	-1.258274000	-0.819347000
H	-1.835126000	1.422850000	-0.503025000

[F₄C₆H₄]⁵⁺

C	-0.657341000	3.533672000	-0.694789000
C	0.767771000	3.588164000	-0.171110000
C	-2.944570000	2.457791000	-0.549905000
N	1.641507000	2.453686000	-0.634421000
N	-1.542676000	2.544888000	0.015956000

C	3.045093000	2.478002000	-0.066099000
C	3.843853000	1.268629000	-0.513554000
C	-3.783625000	1.424874000	0.178675000
C	-3.831946000	-0.499632000	-1.288017000
C	2.964755000	-1.325435000	-2.130051000
N	-1.624659000	-1.246864000	-2.204890000
N	-3.334038000	0.028537000	-0.000484000
N	3.334511000	-0.022284000	-0.005093000
C	0.676640000	-1.963630000	-3.009032000
C	-3.032922000	-1.665846000	-1.839113000
C	3.795080000	-1.123327000	-0.876318000
N	1.559900000	-1.787392000	-1.802914000
C	-0.750908000	-2.373394000	-2.687748000
C	3.807436000	-0.240360000	1.378185000
C	-3.830063000	-0.807856000	1.112602000
C	-3.007357000	-0.716401000	2.383866000
N	1.579335000	-0.695324000	2.438514000
N	-1.613541000	-1.272738000	2.186635000
C	2.975490000	-1.221869000	2.182105000
C	-0.728426000	-1.154514000	3.398467000
C	0.691283000	-1.652776000	3.187077000
H	-0.701042000	3.311343000	-1.762439000
H	-1.106607000	4.520134000	-0.561849000
H	1.226239000	4.513100000	-0.527404000
H	0.810372000	3.616566000	0.919020000
H	-3.398667000	3.445203000	-0.450240000
H	-2.840534000	2.250980000	-1.615176000
H	1.723775000	2.510183000	-1.653070000
H	1.217788000	1.534464000	-0.410600000
H	-1.125164000	1.594239000	0.015184000
H	-1.625620000	2.838634000	0.992845000
H	3.524034000	3.395285000	-0.412600000
H	2.944620000	2.548485000	1.017070000
H	3.864995000	1.239992000	-1.606229000
H	4.886081000	1.441050000	-0.214671000
H	-4.821350000	1.562932000	-0.152505000
H	-3.795390000	1.664160000	1.245284000
H	-3.840490000	0.306649000	-2.026470000
H	-4.877061000	-0.828478000	-1.216924000
H	2.866244000	-0.420665000	-2.730206000
H	3.421232000	-2.089504000	-2.761636000
H	-1.697859000	-0.556186000	-2.956680000
H	-1.205286000	-0.767335000	-1.386606000
H	0.723108000	-1.042433000	-3.592658000
H	1.125375000	-2.746895000	-3.623556000
H	-3.505831000	-2.053009000	-2.743233000
H	-2.942217000	-2.494079000	-1.135997000
H	4.834604000	-0.979055000	-1.198802000
H	3.805988000	-2.054026000	-0.302963000
H	1.143065000	-1.123147000	-1.122328000
H	1.639727000	-2.692798000	-1.332446000
H	-1.206169000	-2.764434000	-3.600141000

H	-0.798476000	-3.172598000	-1.946135000
H	3.832323000	0.718529000	1.902650000
H	4.843687000	-0.602742000	1.401204000
H	-4.865286000	-0.557640000	1.379918000
H	-3.867423000	-1.850834000	0.786992000
H	-2.889388000	0.305194000	2.745529000
H	-3.481611000	-1.293266000	3.179651000
H	1.157167000	-0.421337000	1.530566000
H	1.673048000	0.155847000	2.999083000
H	-1.188841000	-0.808913000	1.361059000
H	-1.710981000	-2.266000000	1.959926000
H	2.861863000	-2.188890000	1.691783000
H	3.441304000	-1.399787000	3.152899000
H	-0.760242000	-0.116331000	3.733900000
H	-1.185299000	-1.753263000	4.189236000
H	0.722004000	-2.611461000	2.666224000
H	1.145722000	-1.813449000	4.166945000
F	-0.000153000	-0.006503000	0.009113000

[F₅C₂H₂]⁵⁺

F	0.003221000	0.001379000	-0.002165000
N	2.609658000	0.033772000	-0.025519000
H	1.542710000	0.018031000	-0.014212000
N	1.140380000	-0.604949000	2.821724000
N	-1.062703000	-0.630714000	2.845370000
N	-2.603820000	-0.033553000	0.024255000
H	-1.538063000	-0.017776000	0.011646000
N	1.045758000	2.767125000	-0.892830000
N	-1.157022000	2.761307000	-0.870165000
N	1.113040000	-2.131266000	-1.961902000
N	-1.089563000	-2.164394000	-1.938175000
C	3.119274000	0.051530000	1.399218000
H	3.005992000	1.067786000	1.773474000
H	4.190981000	-0.152872000	1.352301000
C	2.485058000	-0.935696000	2.380039000
H	2.480990000	-1.956685000	1.996564000
H	3.134409000	-0.957728000	3.258599000
C	0.039019000	-1.104487000	2.322181000
H	0.039751000	-1.858825000	1.551603000
C	-0.732363000	0.292836000	3.954908000
H	-1.129324000	-0.103696000	4.890025000
H	-1.171946000	1.276321000	3.788648000
C	0.812912000	0.316068000	3.933834000
H	1.218146000	1.310888000	3.748208000
H	1.246965000	-0.060925000	4.860466000
C	-2.408992000	-0.989955000	2.430315000
H	-3.040959000	-1.020038000	3.321221000
H	-2.393867000	-2.012456000	2.051373000
C	-3.079659000	-0.016676000	1.460011000

H	-4.149557000	-0.234508000	1.439359000
H	-2.970115000	1.002056000	1.828636000
C	3.074705000	1.275501000	-0.755349000
H	2.960745000	1.089026000	-1.822047000
H	4.144905000	1.372023000	-0.560762000
C	2.397765000	2.596598000	-0.387054000
H	2.391502000	2.774133000	0.689090000
H	3.019516000	3.390119000	-0.808745000
C	-0.048354000	2.559451000	-0.205198000
H	-0.037784000	2.265283000	0.832327000
C	-0.841347000	3.211103000	-2.244367000
H	-1.328241000	4.165177000	-2.446278000
H	-1.197750000	2.484752000	-2.976331000
C	0.698220000	3.327039000	-2.219832000
H	1.177042000	2.769892000	-3.024011000
H	1.037948000	4.362608000	-2.271636000
C	-2.496817000	2.535467000	-0.353551000
H	-3.153781000	3.300072000	-0.774991000
H	-2.486919000	2.722043000	0.720858000
C	-3.125157000	1.185413000	-0.705763000
H	-3.017699000	0.996357000	-1.772756000
H	-4.195935000	1.241622000	-0.499083000
C	3.115312000	-1.202293000	-0.737856000
H	3.032364000	-2.036889000	-0.043314000
H	4.180295000	-1.045143000	-0.921399000
C	2.448763000	-1.567302000	-2.065011000
H	2.416809000	-0.726709000	-2.759233000
H	3.094317000	-2.310950000	-2.538621000
C	-0.000266000	-1.461654000	-2.114888000
H	-0.018404000	-0.417744000	-2.384587000
C	-0.737260000	-3.582465000	-1.698241000
H	-1.154245000	-4.202130000	-2.492789000
H	-1.143041000	-3.929398000	-0.747871000
C	0.807872000	-3.559596000	-1.716952000
H	1.245900000	-3.896758000	-0.777490000
H	1.223548000	-4.165278000	-2.522899000
C	-2.443268000	-1.640389000	-2.009115000
H	-3.078394000	-2.403635000	-2.465251000
H	-2.452561000	-0.801252000	-2.705725000
C	-3.086810000	-1.290761000	-0.666327000
H	-2.955753000	-2.116868000	0.030838000
H	-4.161238000	-1.172015000	-0.821047000