

Supporting Information

A thermodynamic view on the microsolvation of ions by rare gas: application to Li^+ with argon

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Reduced heat capacity and mean Lindemann index plots

In order to facilitate the analysis, the reduced heat capacity (c_V) and the mean Lindemann index ($\langle\delta\rangle$) curves displayed in Figs. 3, 4 and 10 of the paper for both PES I and PES II are shown here by individual plots for each cluster.

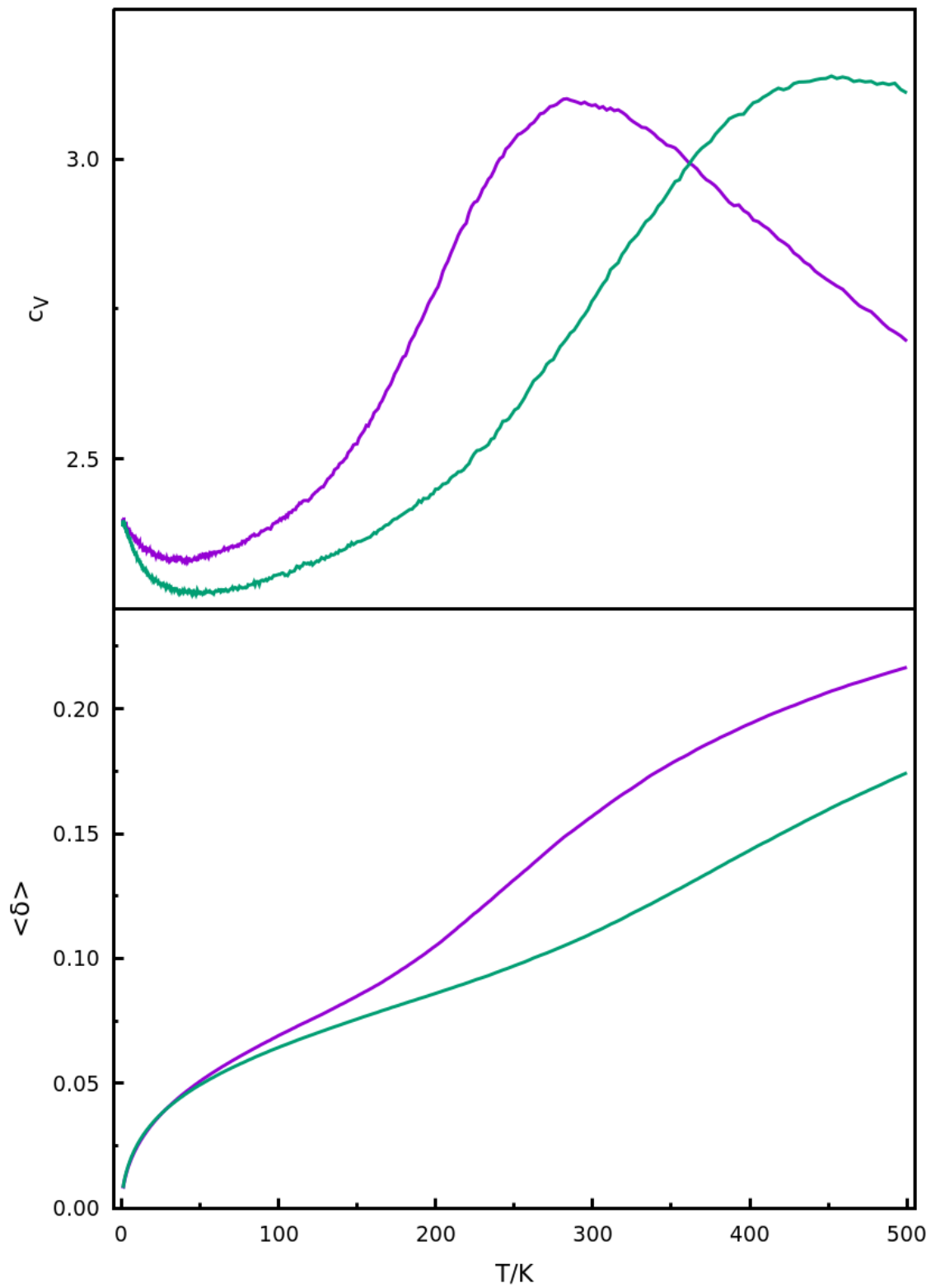


Figure S1: Li^+Ar_4 reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

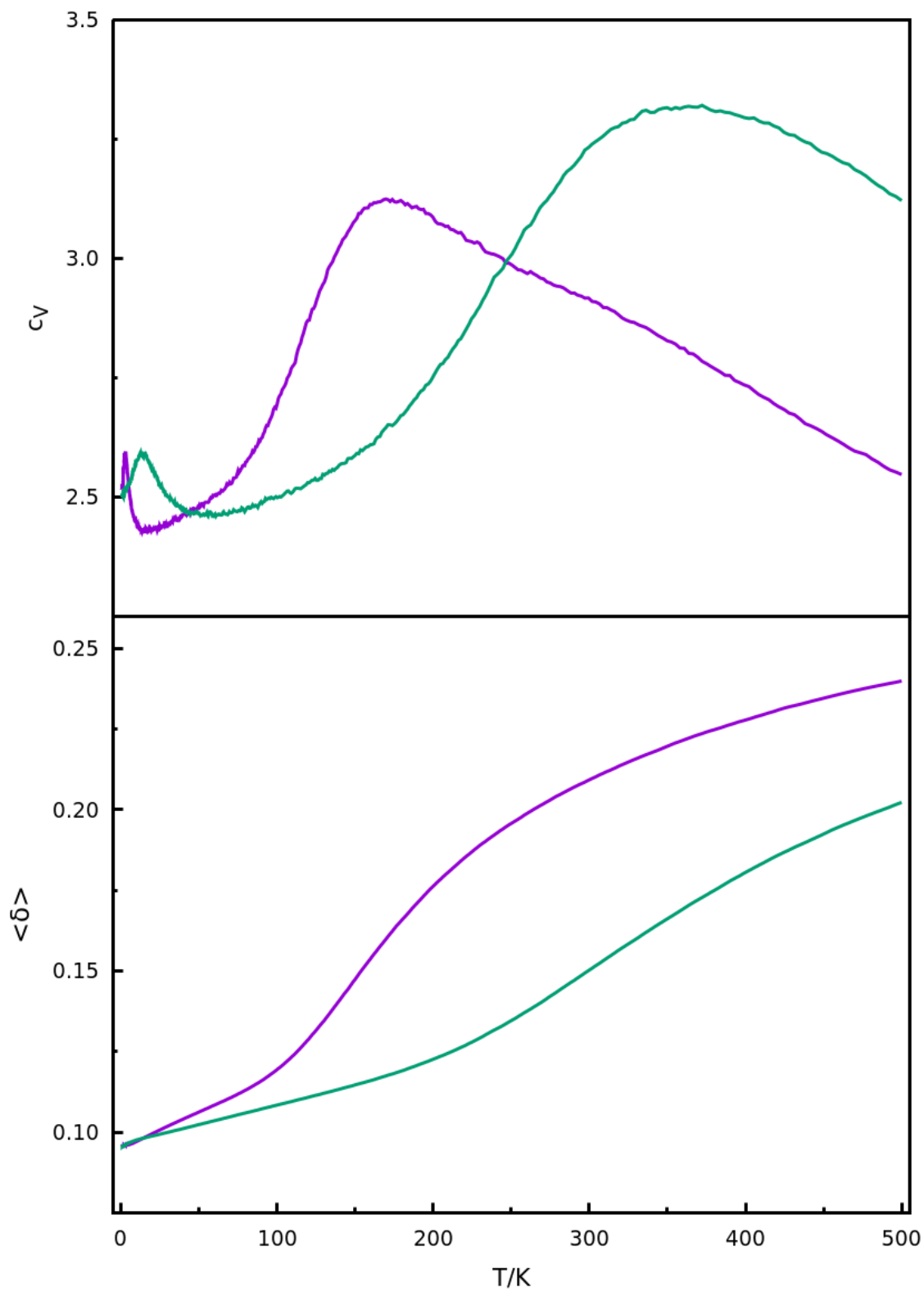


Figure S2: Li^+Ar_5 reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

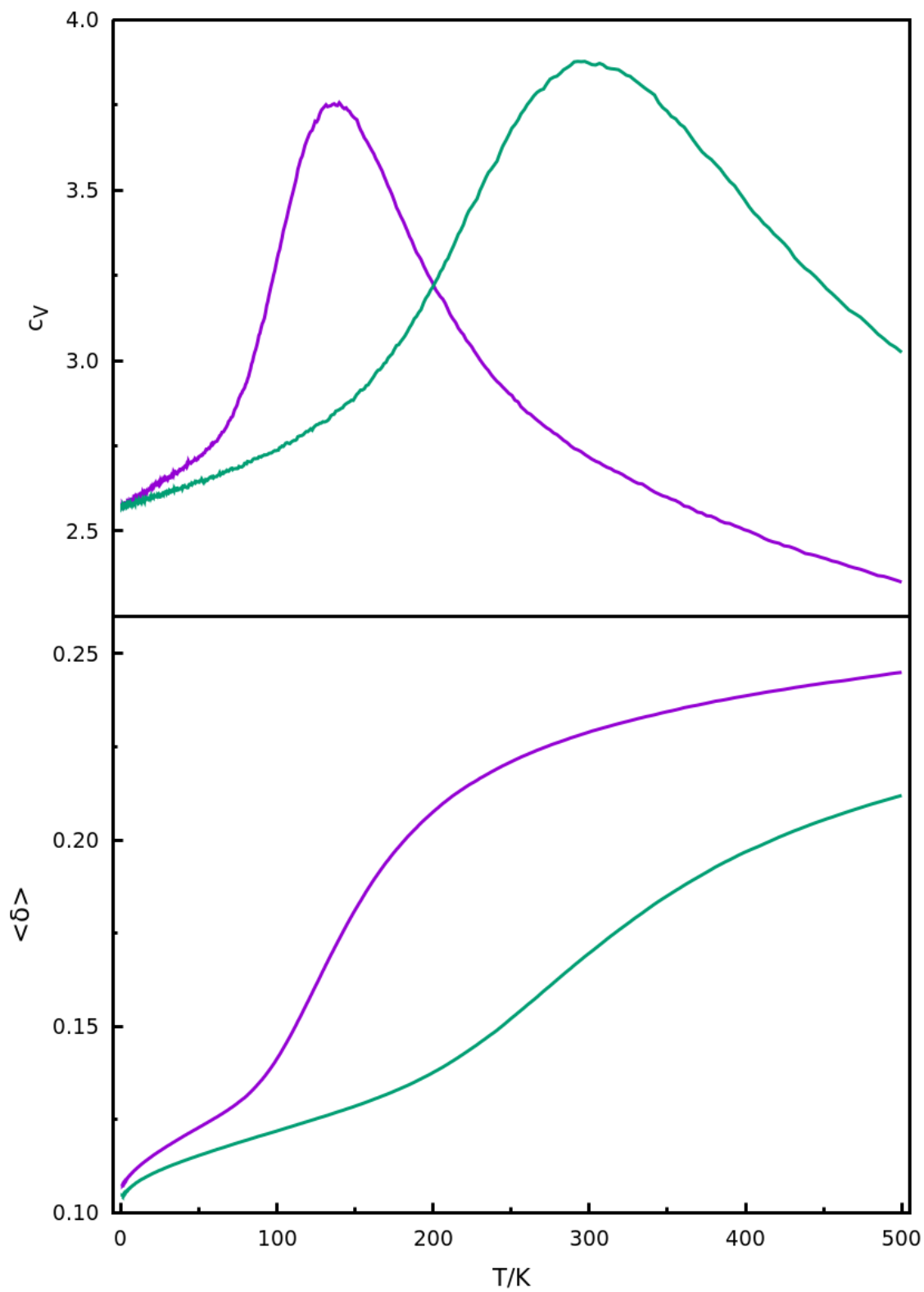


Figure S3: Li^+Ar_6 reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

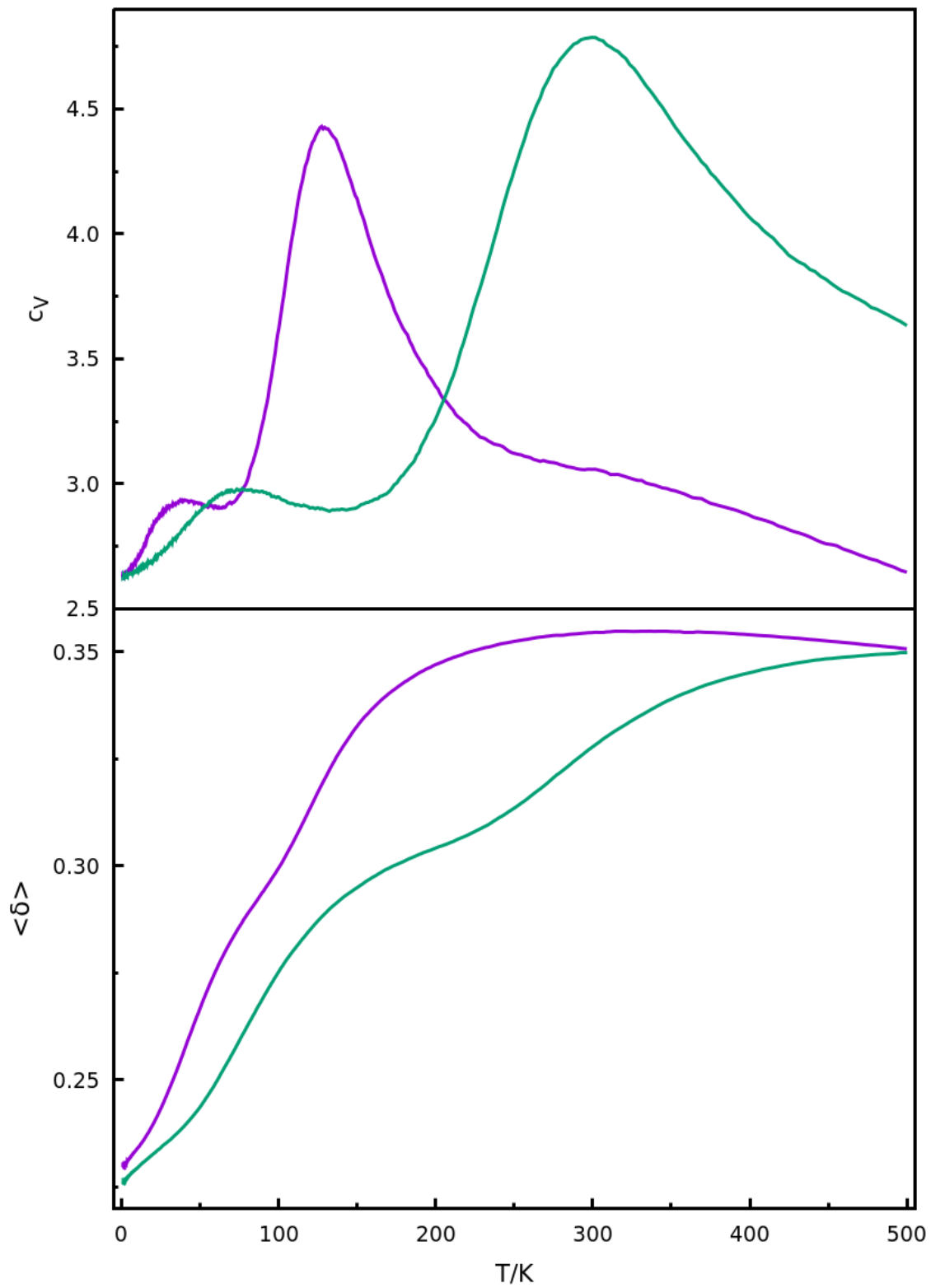


Figure S4: Li^+Ar_7 reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

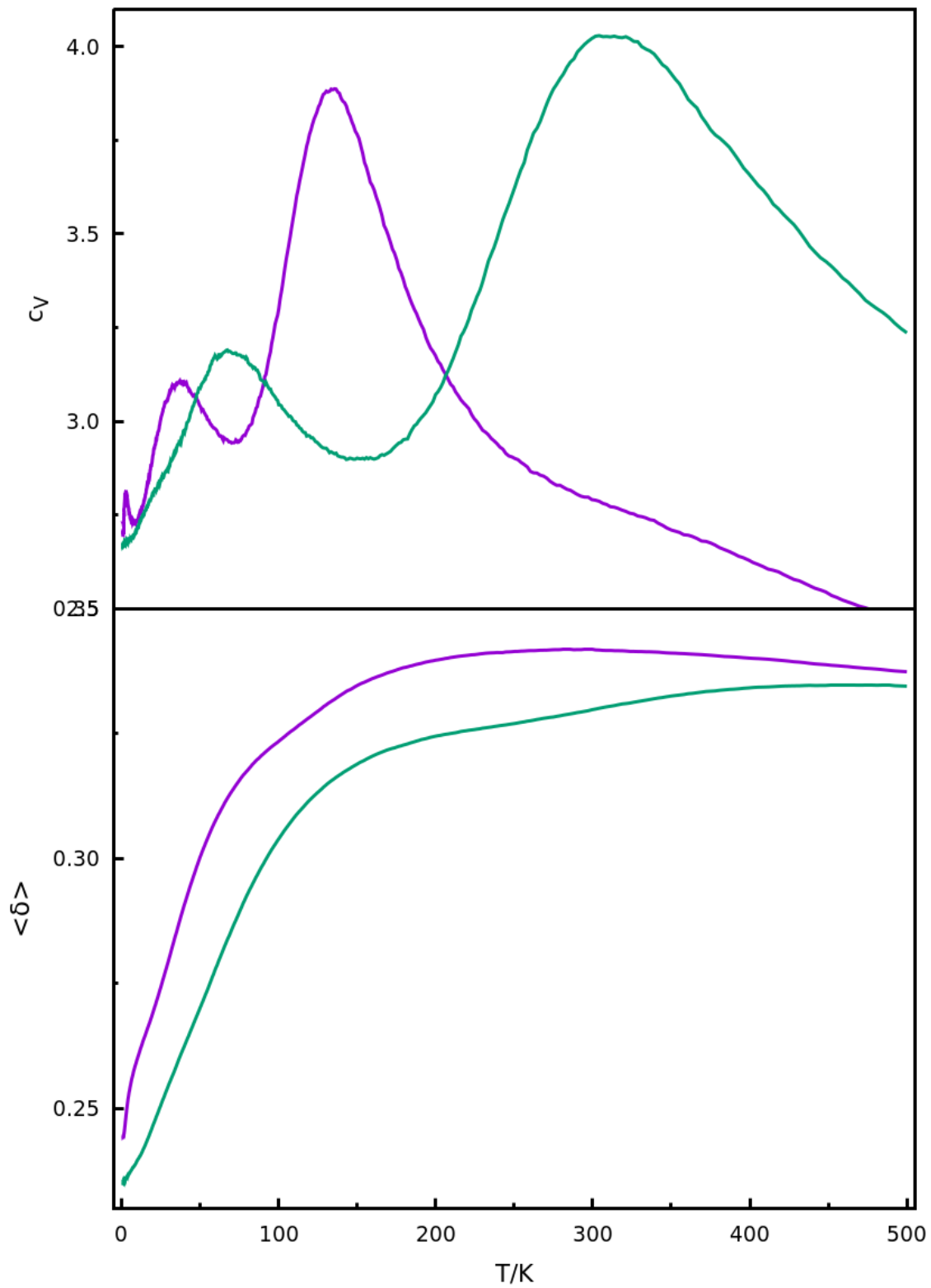


Figure S5: Li^+Ar_8 reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

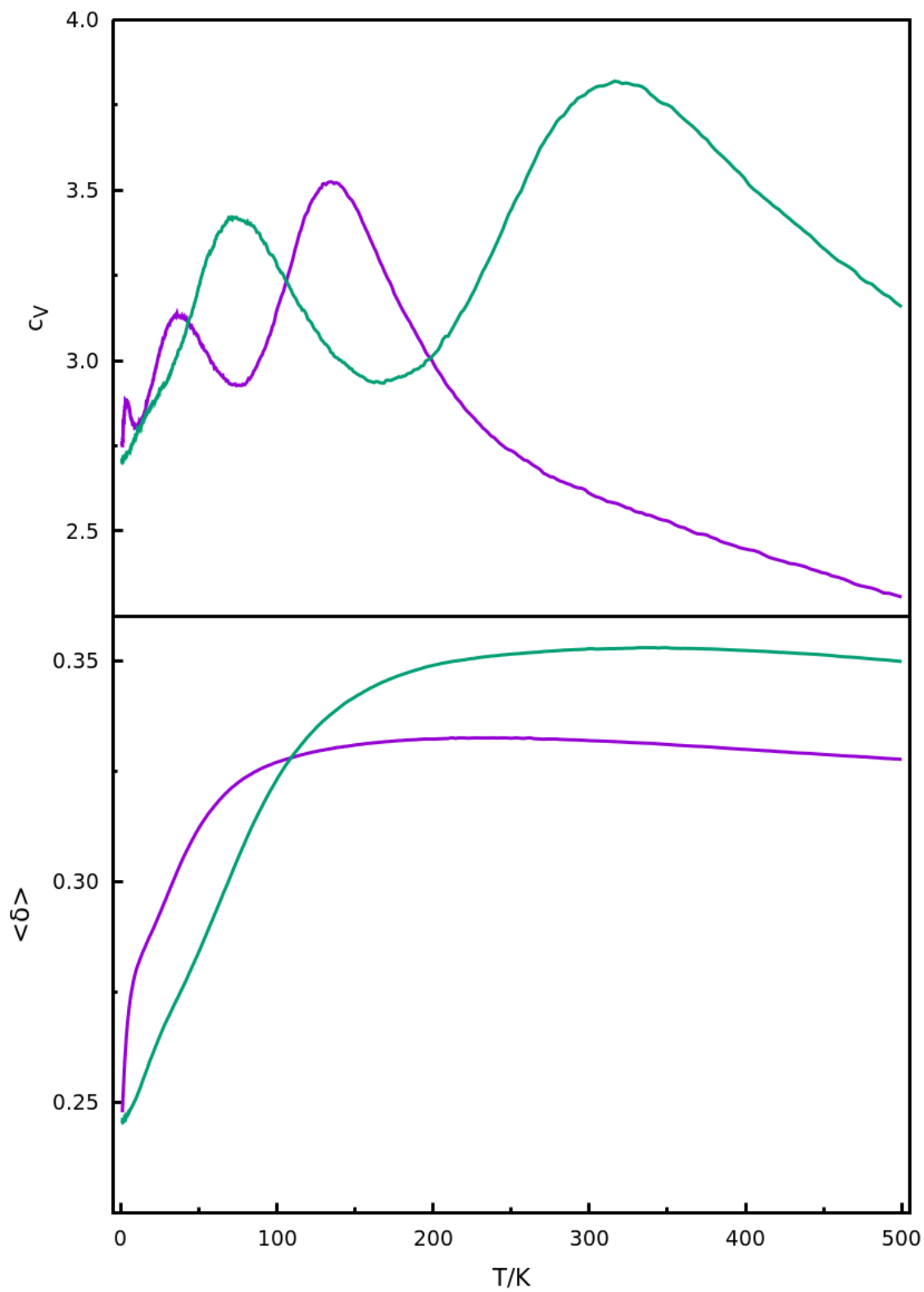


Figure S6: Li^+Ar_9 reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

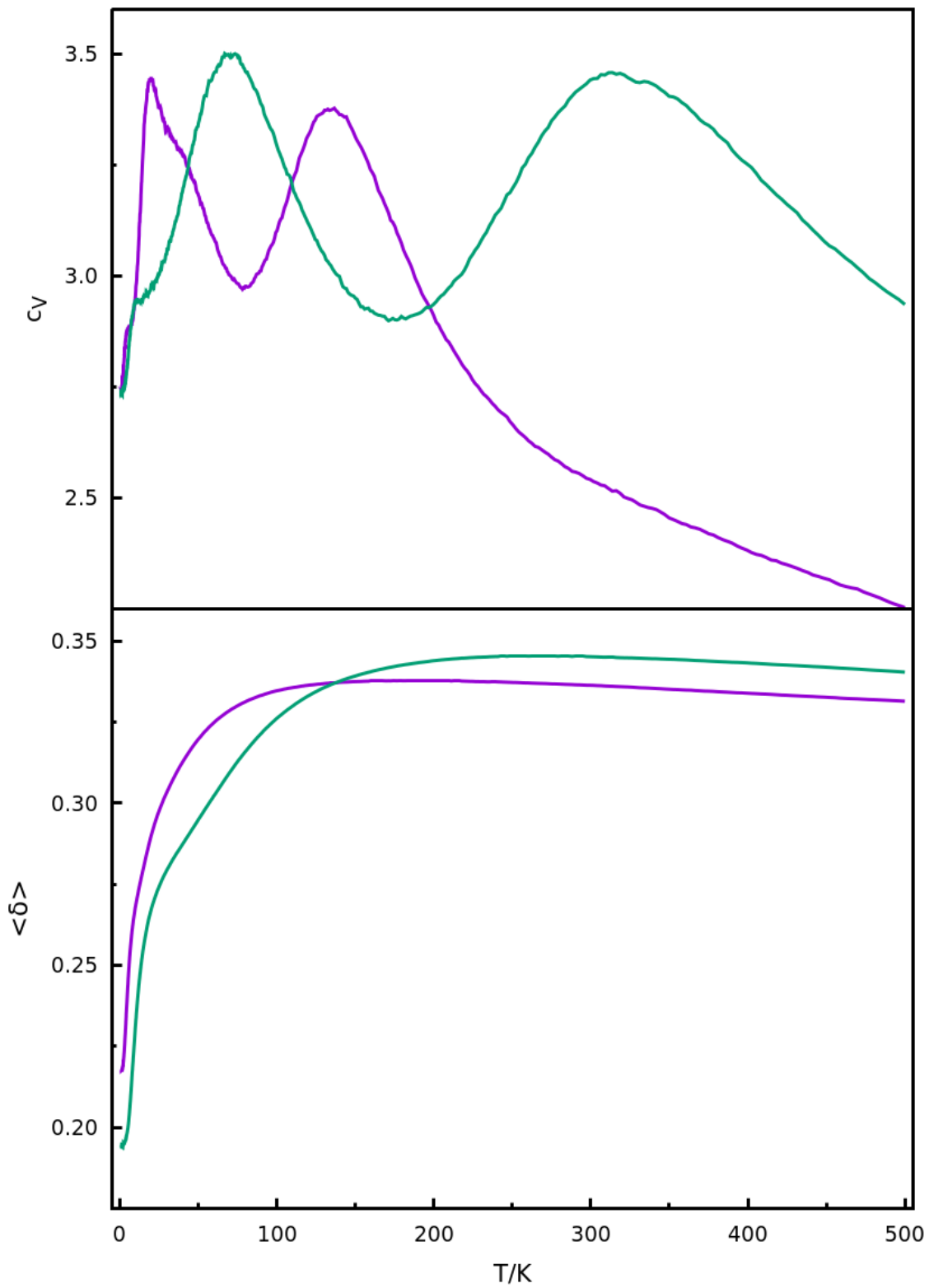


Figure S7: $\text{Li}^+\text{Ar}_{10}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

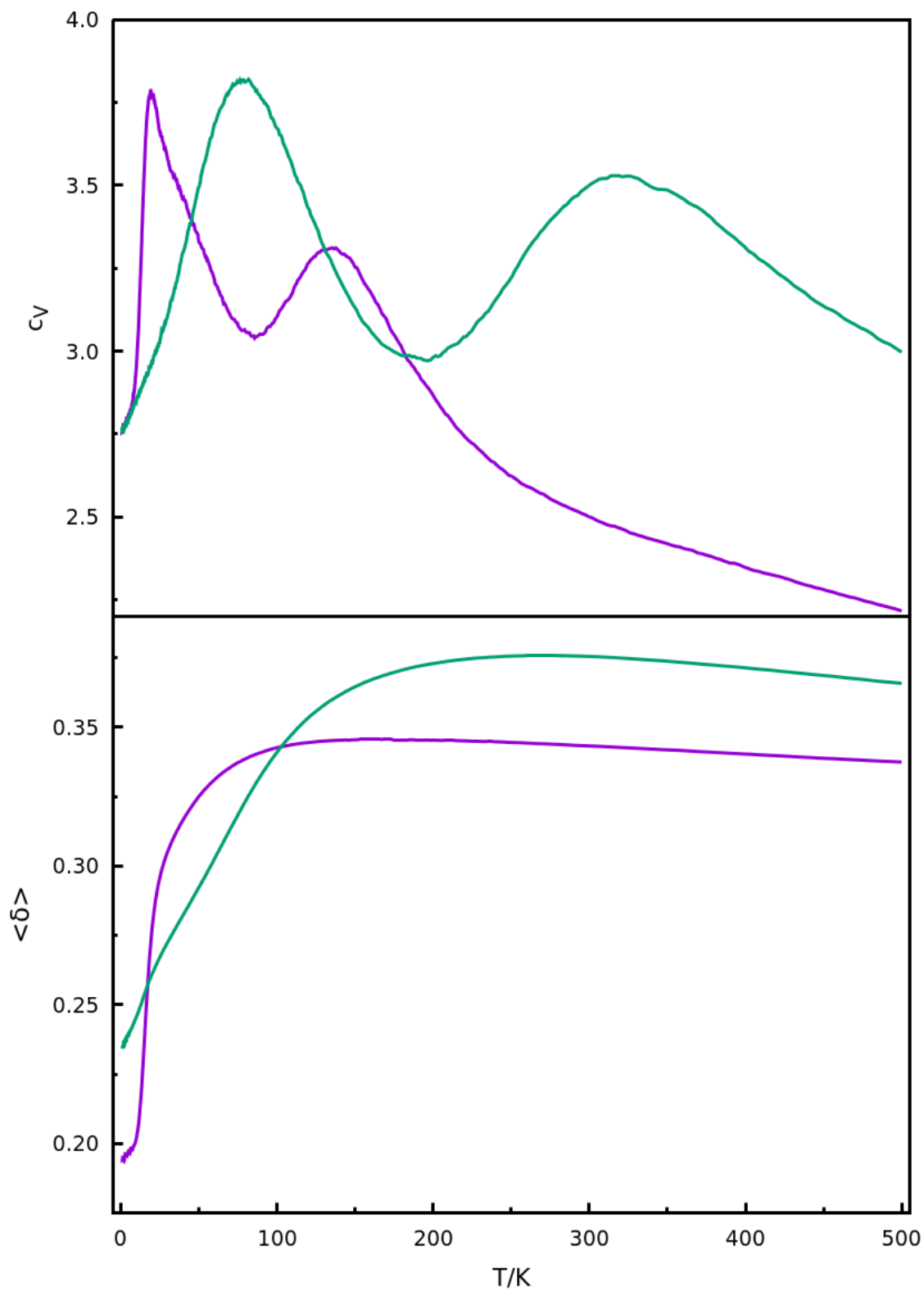


Figure S8: $\text{Li}^+\text{Ar}_{11}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

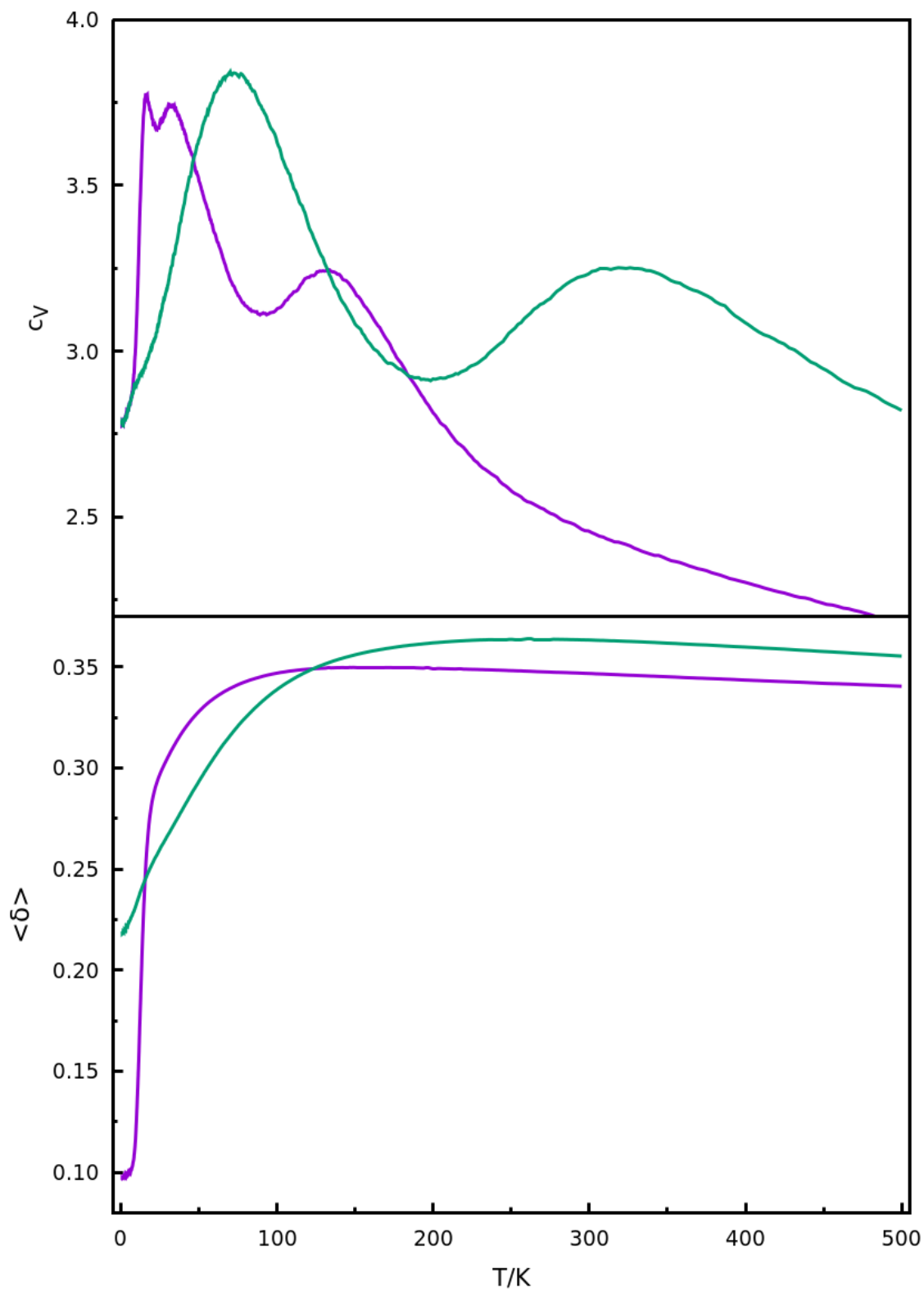


Figure S9: $\text{Li}^+\text{Ar}_{12}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

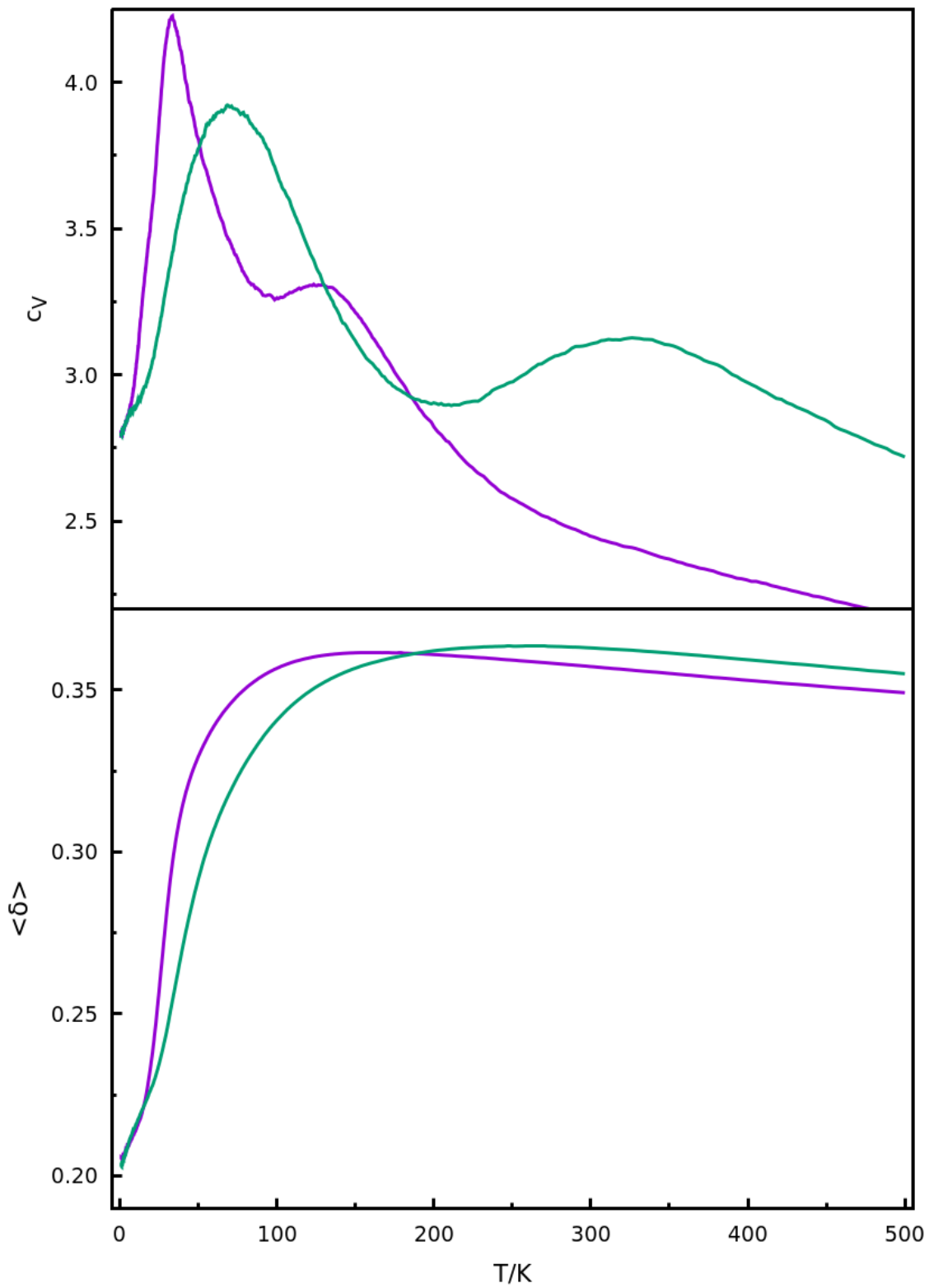


Figure S10: $\text{Li}^+\text{Ar}_{13}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

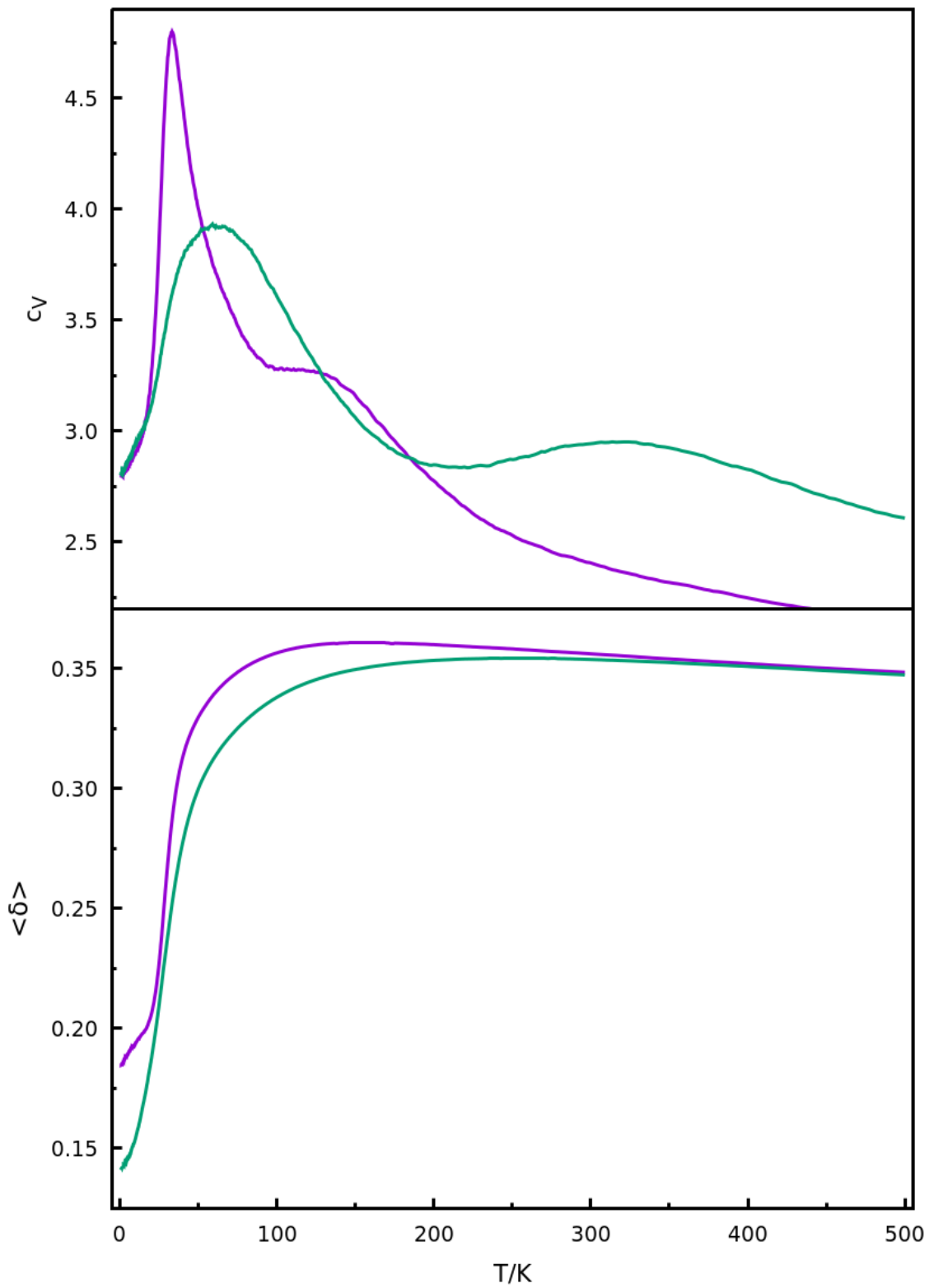


Figure S11: $\text{Li}^+\text{Ar}_{14}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

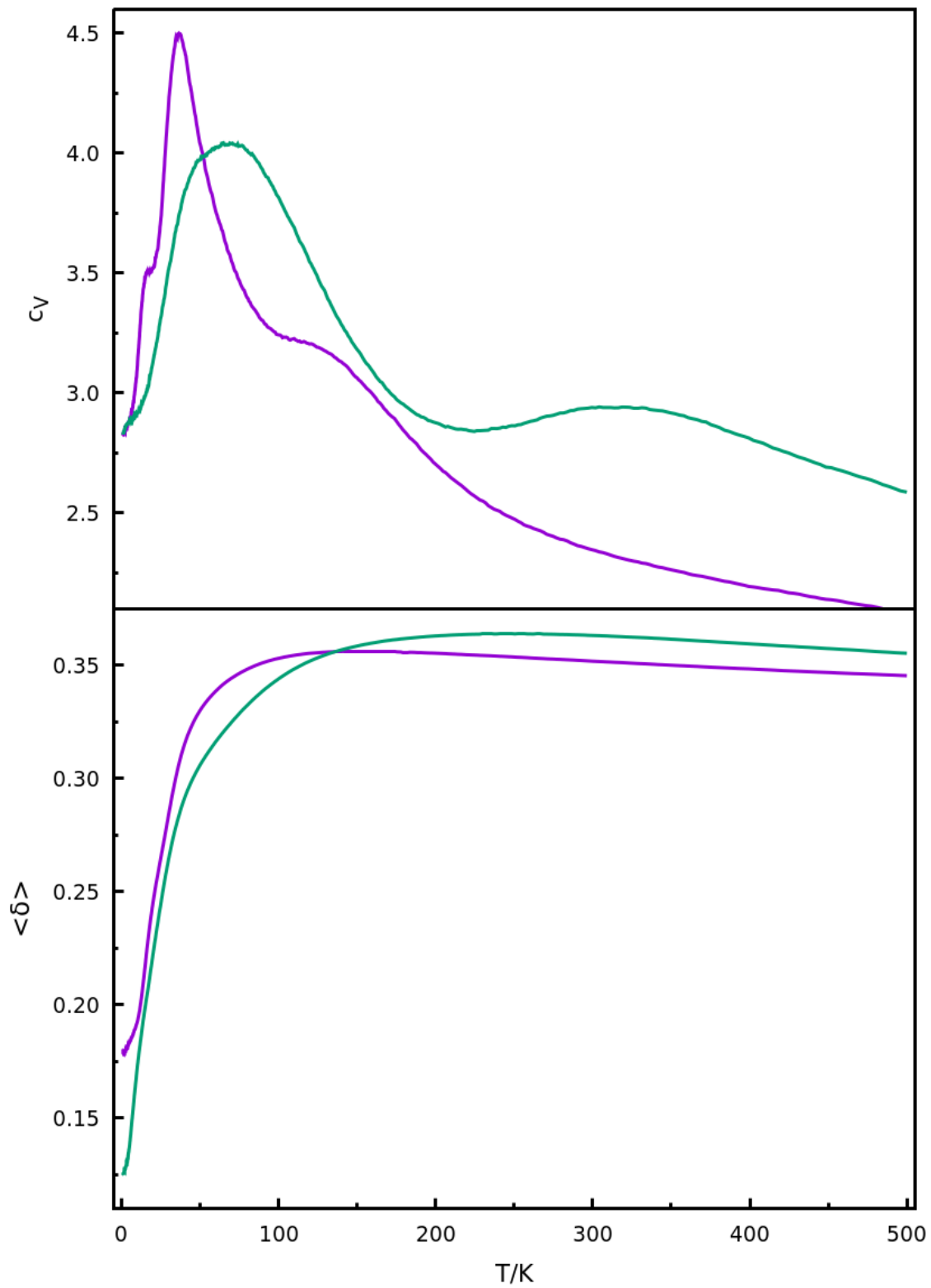


Figure S12: $\text{Li}^+\text{Ar}_{15}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

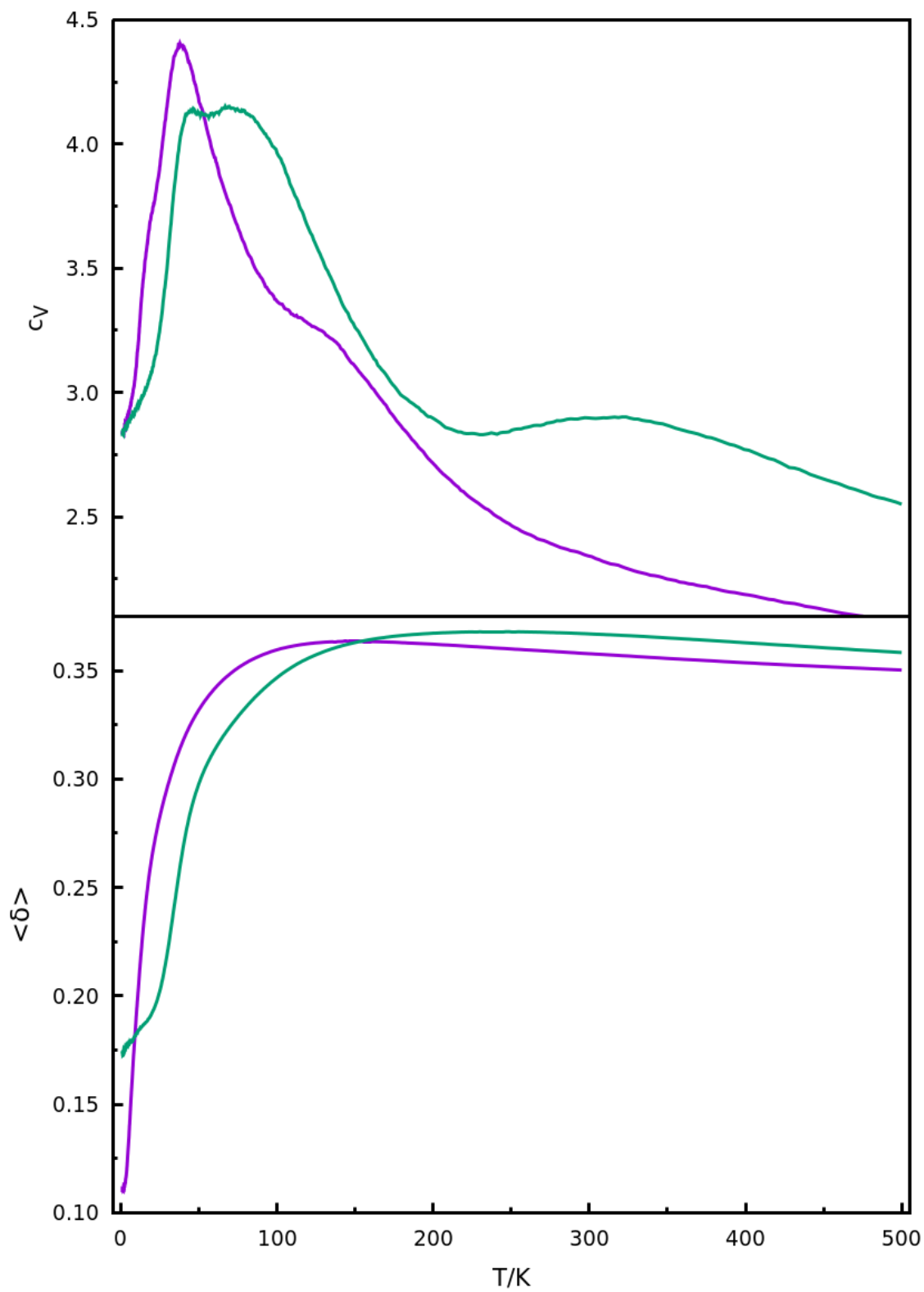


Figure S13: $\text{Li}^+\text{Ar}_{16}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

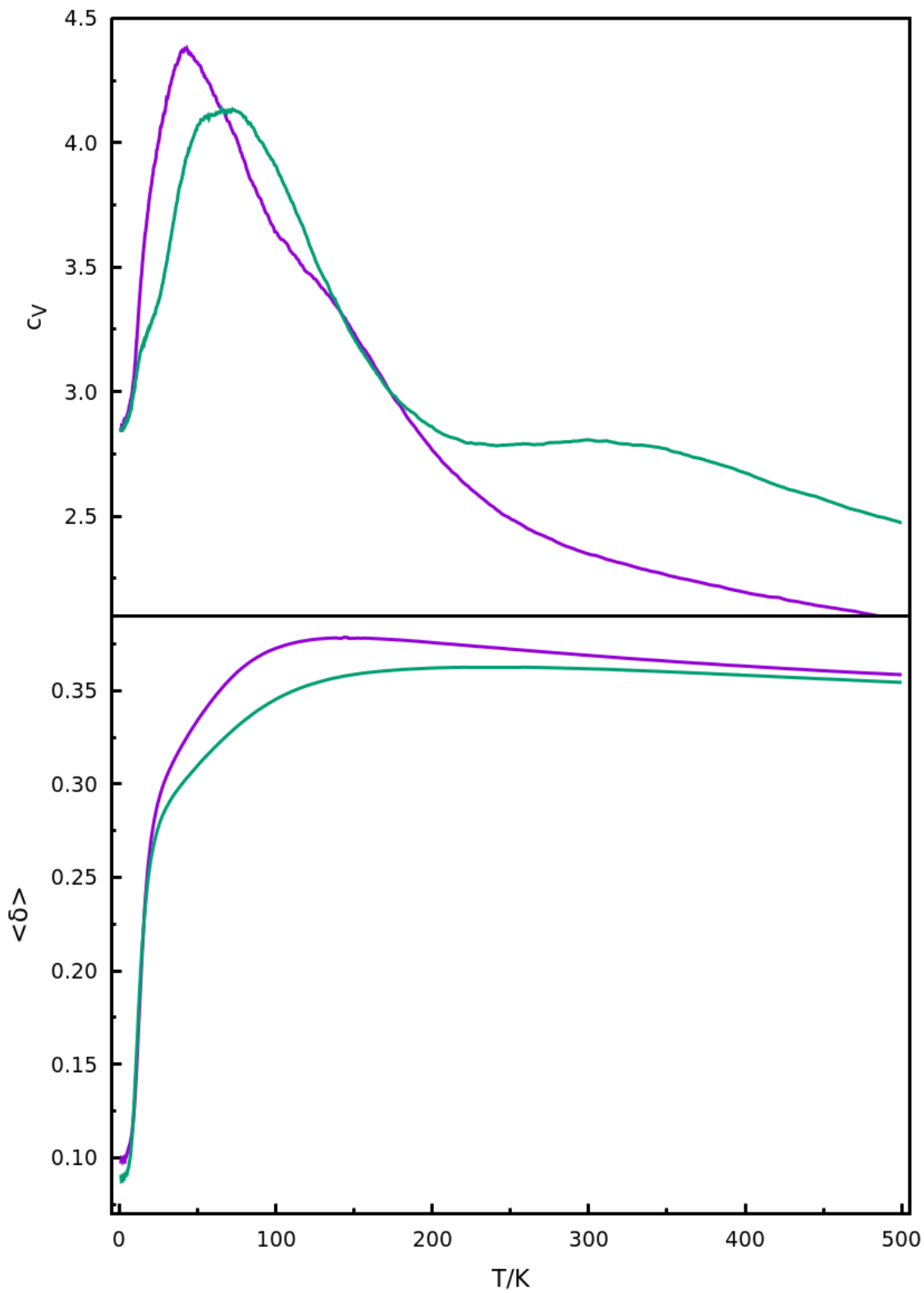


Figure S14: $\text{Li}^+\text{Ar}_{17}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

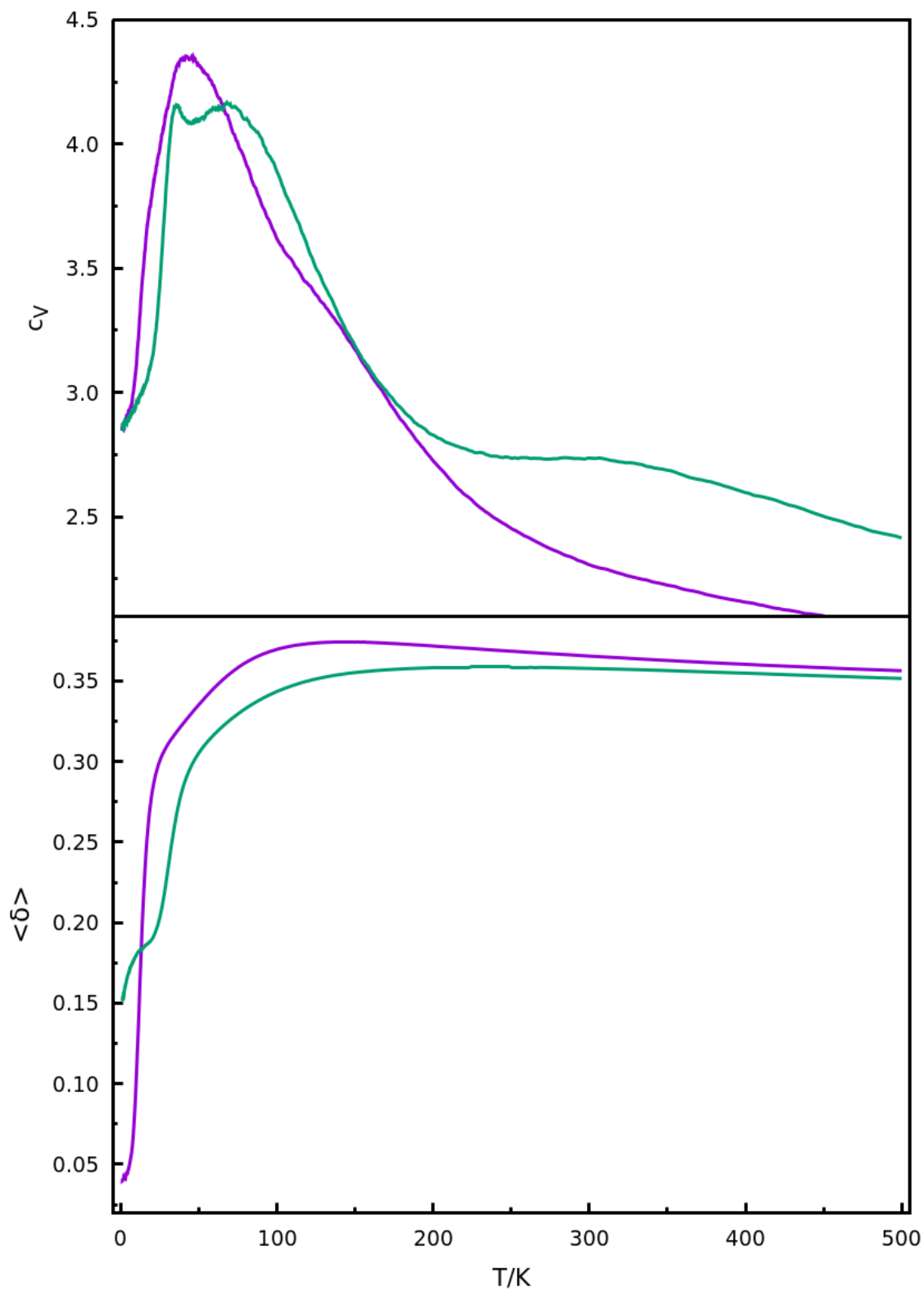


Figure S15: $\text{Li}^+\text{Ar}_{18}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

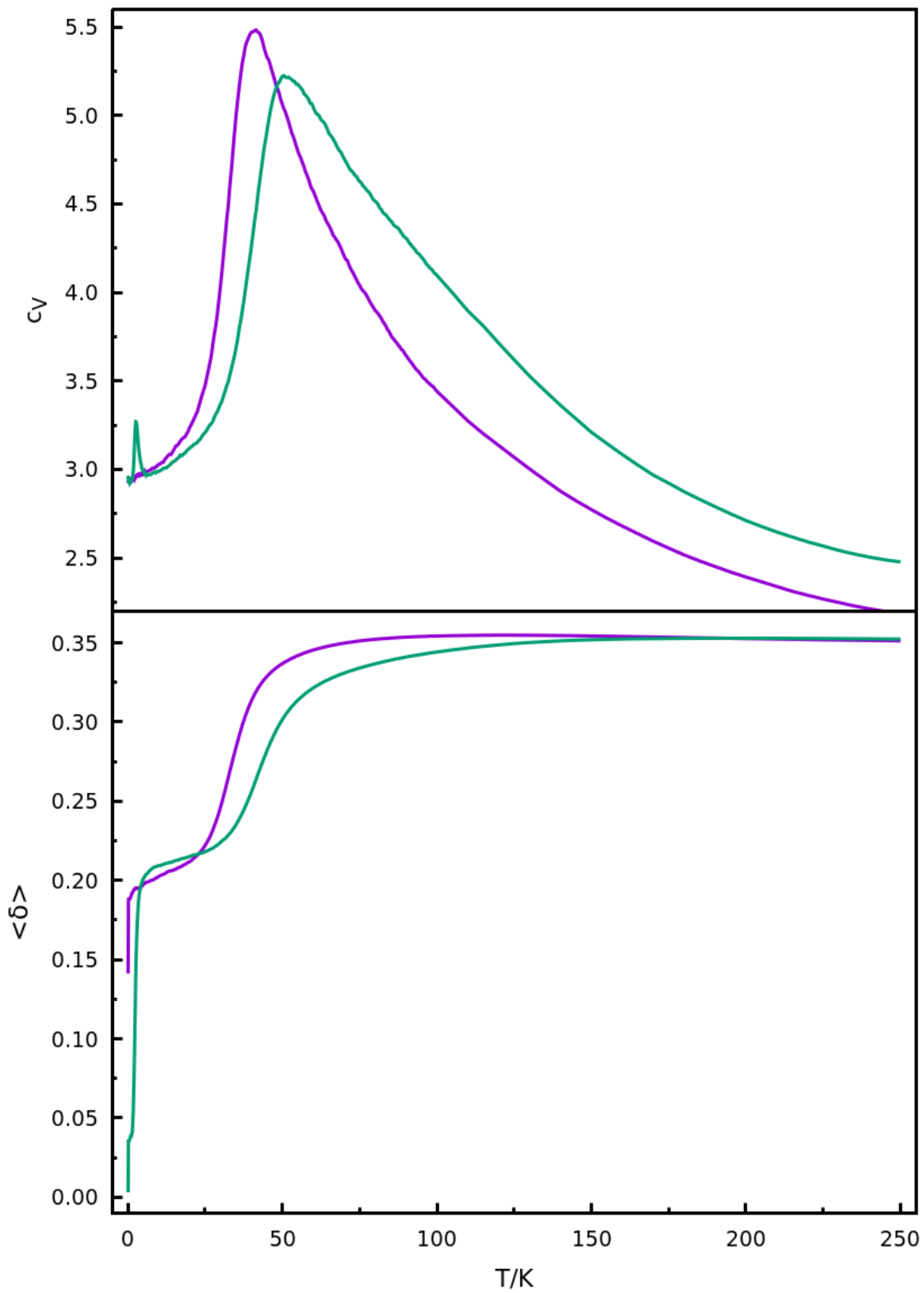


Figure S16: $\text{Li}^+\text{Ar}_{33}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

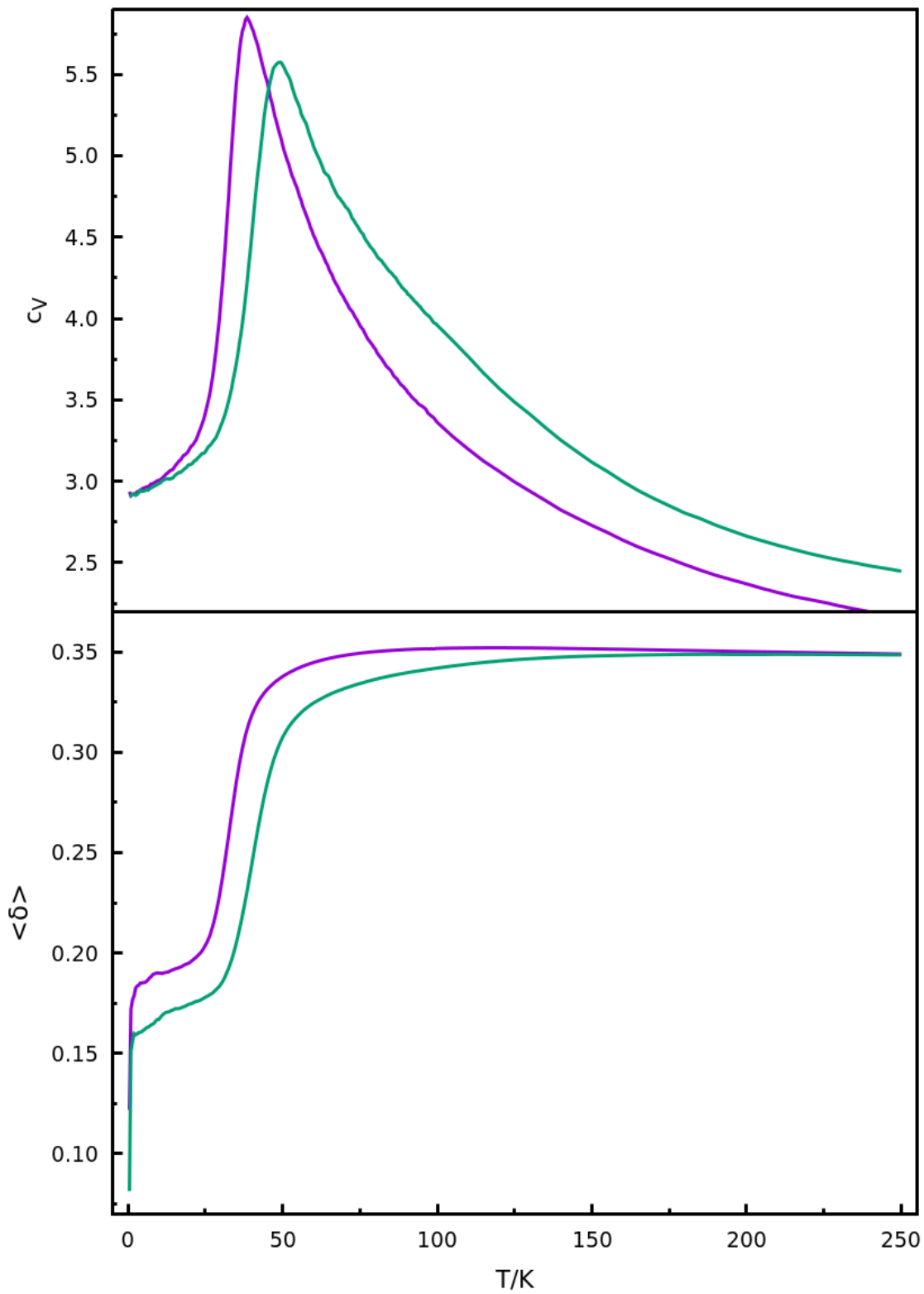


Figure S17: $\text{Li}^+\text{Ar}_{34}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

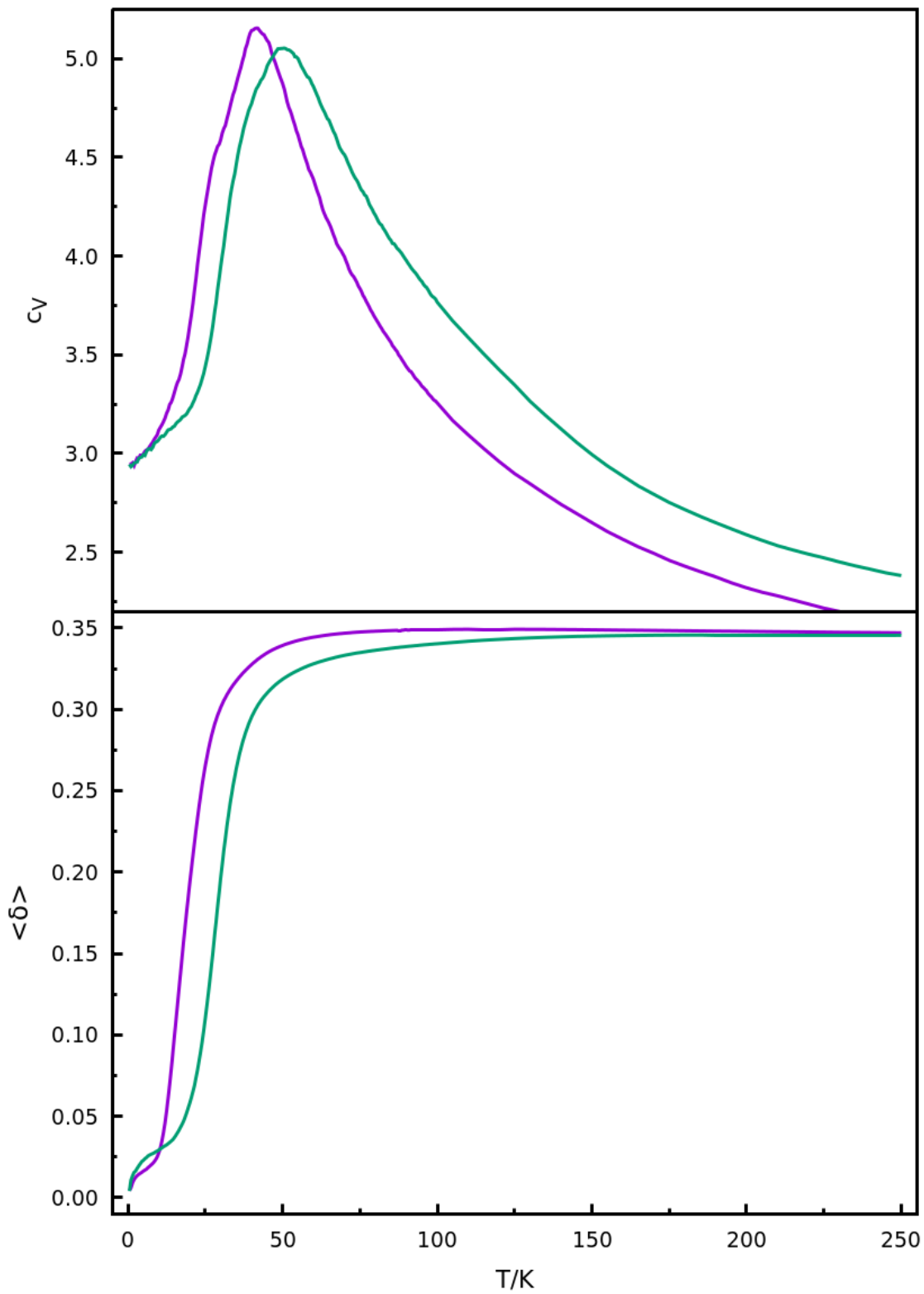


Figure S18: $\text{Li}^+\text{Ar}_{38}$ reduced heat capacity and mean Lindemann index modeled with PES I (magenta) and PES II (green).

Cartesian coordinates and energies of the structures displayed in Fig.11

All coordinates are in a_0 , while the energies are in E_h .

$\text{Li}^+\text{Ar}_{33}$ cluster of PES I

Structure corresponding to the green curve:

34

Energy=-0.10669443487108157

Ar	11.382555002573685	5.6913650500727622	5.7663093877126634
Ar	6.0815818078196759	15.634567772601065	18.497530056770398
Ar	16.133825472382412	16.207444590561426	11.926233342350434
Ar	6.0962797554877008	10.213906660735553	8.2974180402756339
Ar	10.784093753227676	8.3675838993410512	13.254596155989971
Ar	14.126456830988788	12.750624935518463	17.299915454272323
Ar	14.199908462742986	2.7195185457440334	11.668231558463402
Ar	6.6601427279434073	3.5382453214863876	10.619629587535394
Ar	22.835564823812756	16.118629436521786	12.644884064749354
Ar	21.293586505896069	10.696679693439572	17.523246892034980
Ar	15.771486382427442	10.028568806186318	1.7926819816331534
Ar	9.4652420748850457	14.923914884795867	12.733758237630012
Ar	9.1229189245755169	9.3200852974421231	20.387519191379003
Ar	12.396119909719895	21.291430657974775	9.5135602811958524
Ar	17.320968329298374	9.5049760397901402	12.205299047386392
Ar	9.0401124631515071	11.873928580632104	2.0634478687146922
Ar	18.691198586170824	5.8032352820927571	6.7640770919112576
Ar	12.870405265882418	11.955954077972320	7.7851611843353332

Ar	20.876863182225271	3.9094358203784640	13.876307761738664
Ar	11.760941477603822	15.830010449521845	22.878221637023014
Ar	24.049325675547706	9.3320323375094887	10.756395882188361
Ar	19.756896159791371	13.168221486822203	6.6540293643690189
Ar	7.4299421311346006	17.099837070134669	6.6136313777368398
Ar	19.442862170732646	20.185610425107445	7.3520727838675164
Ar	9.0549814320192503	2.9952690730606442	17.164665999470941
Ar	12.320083236282446	19.714346287913095	16.869733841644820
Ar	18.950406104272624	17.433298461043126	18.602876588754910
Ar	14.158350286199097	17.134581058742494	3.6875492792736293
Ar	15.477356649302894	5.9480369550869021	18.086486108082013
Ar	18.179309549785167	22.524618498259201	13.815380197134845
Ar	6.3307817615072182	21.003390173351807	13.207730119795297
Ar	4.3228224915230680	9.1198589264590826	15.180314873596108
Ar	2.6134594272070557	15.205545694457220	11.938281860341622
Li	13.450868425925089	12.284478513648843	12.539678975717107

Li⁺Ar₃₃ cluster of PES II

Structure corresponding to the green curve:

34

Energy=-0.14041354257219510

Ar	12.188763241683922	7.9592388491002435	9.82306440923754950E-003
Ar	17.702137840548136	8.5024359970035643	4.0745651313466009
Ar	9.6057835861735850	14.082334361999223	2.6706076339111116
Ar	5.9137892395973708	8.3199547728848735	2.6930847803894435
Ar	9.6062864518594253	2.7487060723679235	4.1828786240669560
Ar	15.143269091697674	3.2938142751625037	8.2645922491742621

Ar	2.4892810113125425	14.251443744217251	2.4045466060843070
Ar	15.142573366898409	14.627040259990274	6.7531759481506448
Ar	11.295024874771837	8.8825366457919781	6.9061155052318108
Ar	2.4832295820626626	2.5246188689381479	3.9634206914881096
Ar	16.913509379865101	9.4023490468900057	10.803254751375128
Ar	9.4190170205968915	18.272508037720637	8.1968966312410867
Ar	0.21853572733669865	8.8236015285969316	6.4229409874633481
Ar	2.3381582291682506	18.420156140106577	7.8755994203840425
Ar	9.4134231271090982	0.15482894266418129	10.624025373780453
Ar	5.8965407899457851	5.8679605396101522	9.0969568952075548
Ar	17.428600140766200	3.9948068362208029	14.981851975727441
Ar	2.3257756130176146	-5.13003260613128162E-002	10.342340243775260
Ar	5.8914240490846206	12.358761936457693	8.2405039873460861
Ar	11.141736909365713	12.875453376111523	12.111572000270529
Ar	11.149683938204820	6.3850061685109241	12.970192742741997
Ar	17.420493718571294	15.720774094684959	13.413558864523047
Ar	11.741841244342680	19.345828358152232	14.808763852943544
Ar	5.5271549656588848	3.1837406931287275	15.489599815839490
Ar	5.5414969405977921	16.620821131681456	13.676789507490700
Ar	5.7805407023980271	9.8347031317346492	14.258231985419407
Ar	14.946553939226495	10.272443351887986	17.282125246022911
Ar	4.15469815276970772E-002	6.2181930698083416	12.810563581187475
Ar	4.23415220878206253E-002	13.040113963392951	11.900911508654149
Ar	11.744183007062279	0.87664183453077915	17.287814734721277
Ar	9.2631857692511002	13.947783909646514	18.698915064183847
Ar	9.2626166790395583	7.1263390421902661	19.610278681129337
Ar	2.0912599366187608	13.194293923018453	18.814776963802878

Li 8.5403080752019793 9.3688220163603315 10.577416011086894

Structure corresponding to the blue curve:

34

Energy=-0.14035529731798596

Ar	12.690465863297410	9.5858361606692704	0.68247891859462362
Ar	17.617563224725995	7.1834940325540781	4.8681668594884693
Ar	9.0217444087712462	14.903065496441162	3.3607502193596779
Ar	6.3589520483488338	8.4531658048728495	3.3743389744651151
Ar	11.313912304047943	3.4856194541858603	4.8124620711203683
Ar	16.095337786873614	2.7763328355134242	10.090515241344894
Ar	1.7951881684734035	13.721008836827149	3.8411819691488005
Ar	15.746818288615305	14.352294643319008	5.7269882846605160
Ar	11.659667633950287	9.4741161666237197	7.4689935387589088
Ar	4.5103588717003085	1.8747550229209067	4.6910153753064616
Ar	17.298331594349253	9.8597553945490901	11.234029754892756
Ar	10.823853575810530	18.363257618161992	9.0360933397539505
Ar	0.50556718759972163	7.7753716130353308	7.1894166896237595
Ar	3.9740385017484079	18.923352031463715	7.8063001758494162
Ar	9.4148054434119590	0.23973088145034549	10.610404927820131
Ar	6.4033700167338461	6.1175254249789690	9.7205046588383102
Ar	17.572892543526081	5.6972400060065675	16.774246505073680
Ar	2.1277193402273116	0.91635306769836344	11.098471727912170
Ar	6.2344043463767003	12.551873766195836	8.9537700187264271
Ar	11.546805487425454	13.074996972787369	12.857659271683028
Ar	11.726588767977505	6.5707774138753035	13.265038559294307
Ar	17.332702443719548	16.736041828956651	12.092723147645623
Ar	12.264646210651664	19.111958339076086	16.117744819219926

Ar	6.3384248983211426	3.3958372316161749	16.091533996879932
Ar	5.9415375142010687	16.804977692497069	14.140543712915301
Ar	6.3712968217775652	9.9832781655418419	14.983408789847269
Ar	15.808562589205861	12.365719292879144	17.858585900844531
Ar	0.52898021042201271	7.0088606367912982	14.071510634933816
Ar	0.23026058043383102	13.507259493153310	11.494885700501438
Ar	12.774508672285197	0.73881616960411134	16.714607287181462
Ar	9.1257447924919504	14.008819231090833	19.615633510511930
Ar	11.020442048670699	7.3507251853361781	19.761770551421897
Ar	1.6136330192514790	13.205166347186671	18.453430953676360
Li	8.9808083715780445	9.6308774334725520	11.202516289028273

Li⁺Ar₃₄ cluster of PES I

Structure corresponding to the green curve:

35

Energy=-0.10937779398554232

Ar	13.854218193244101	9.9520667177857955	18.489541992001097
Ar	2.2262710425533649	15.505675232898300	14.607656385668232
Ar	17.810985861446536	12.749601941075829	13.757610128910144
Ar	12.607338723920643	8.8251911177594344	11.938336980304147
Ar	8.8079679587393223	9.7573418809262424	22.942771221012663
Ar	12.122581155628756	16.201094048418138	4.0221037615214046
Ar	13.621321541343702	16.623635918866725	17.393334859400582
Ar	12.365277292884940	15.499942718596342	10.834009692579006
Ar	19.788313159693796	6.7770552139696774	18.658417485271730
Ar	16.157390179312095	9.2564155575016773	24.906667689273934
Ar	6.5047987290283888	16.369650875022732	20.883164877880315

Ar	21.016194343534998	18.526724957322113	15.052353583507980
Ar	13.374315009039377	3.8073463894804913	21.487599385186051
Ar	15.069906784573103	4.6440506616724893	7.1010200506465129
Ar	10.808879815504174	21.646687839244358	8.2359812104704098
Ar	3.0361987001985646	9.9175848701350819	18.762164685134206
Ar	7.9617186684668617	19.707866378851936	14.458589054163202
Ar	19.351116368947238	13.906620109738858	20.575418051661167
Ar	8.4114430981872399	12.712900323821430	15.560037292544576
Ar	13.046663992573924	15.608337910821202	24.024616988152051
Ar	17.719214137509187	20.817544987965409	20.942982082071893
Ar	8.4245212801327405	5.7327084497434440	16.756961921002965
Ar	24.220262603605029	11.640186054439313	15.915730112368358
Ar	14.970206953051612	3.0985558681443686	14.576576669517630
Ar	20.278912689980828	6.9506079625403929	11.382521436480852
Ar	8.8229030770645682	3.4350801436829750	10.041046430430413
Ar	10.826380112033272	22.027983545887775	20.544377736126997
Ar	14.861637692538753	22.339114954499340	14.058102482888708
Ar	16.710732709137421	11.561400160457319	6.8520720507971644
Ar	17.823753059566538	18.672067189933315	8.4910135211802729
Ar	22.967381643872365	13.816918235794731	9.3718893280796252
Ar	9.5756254235213021	9.8496220910655676	6.0132949580156332
Ar	6.0232693859917790	15.684304799263343	8.5790626287058664
Ar	4.6456974357182483	9.0625525578681803	11.339861144219446
Li	13.111827466605826	12.727258741564770	14.662297589257115

Structure corresponding to the blue curve:

35

Energy=-0.10896789303938988

Ar	-3.8708709030352697	25.350716008061415	14.241654706666630
Ar	5.5698804523132308	17.326283237064814	5.8735123452498463
Ar	9.2335323338560205	23.062273178015946	12.080518168704002
Ar	-0.17429991459010805	14.113415561567475	9.4556660041057832
Ar	15.923018219344918	16.395270666526770	15.892483210091166
Ar	0.41364922023320344	31.235617477408368	14.710397654700319
Ar	9.3880482226916122	18.580512551779631	17.193614626795192
Ar	2.7804445660234967	24.559772394638561	13.630521859791894
Ar	6.0845805972401132	14.749916596098354	22.196902718585044
Ar	8.7978865483553790	21.061010753249960	23.813645121994170
Ar	2.5018910052728631	13.003686231404187	16.393569255689318
Ar	11.222524211335623	16.388223083738929	10.770047599608183
Ar	-3.6895634958458903	21.978861659788222	20.614776406048975
Ar	1.1260791990960362	26.921087798117895	20.078772117556785
Ar	5.5241767665063124	24.564284467445791	6.6003167654995192
Ar	6.4690632268393262	31.768708927230087	18.460563400393202
Ar	-0.18897950911649389	28.196890057532659	8.5120496424800898
Ar	12.826523271217470	28.411872936147692	15.016540265824560
Ar	3.0565705444177578	20.169526870334163	18.841245138644894
Ar	14.449213839012387	22.699368021969264	19.120216070083540
Ar	6.2268422052760073	11.580972896195204	10.447095083475872
Ar	1.8422884044036549	21.871272971601144	25.290705503229457
Ar	11.719538557481462	21.108814822987519	5.7450096068184235
Ar	13.126058798888680	15.693150216786790	22.221372602284124
Ar	12.371716358524122	27.656593912287352	7.9768960400610878
Ar	-2.1881145667282573	18.321304657835835	14.794498500522012
Ar	4.5623843548981435	18.157148253337230	12.473995314141197

Ar	6.6547101693654547	29.789999289275066	11.545702164270816
Ar	6.4052673089136904	27.699192936927023	24.618550377381407
Ar	-0.99767777298574534	15.673625026102888	22.016832337347189
Ar	7.7121542229732496	25.116264531437228	18.320601523299953
Ar	9.9083022975408337	11.904847993422308	16.585369546315718
Ar	15.896308534225856	22.309057079208110	11.843503156908735
Ar	-0.44401748065629532	21.115323197102725	8.4643050797966257
Li	6.1173696299904634	21.606867592633169	15.427001022075050

Li⁺Ar₃₄ cluster of PES II

Structure corresponding to the green curve:

35

Energy=-0.14344391599442957

Ar	17.630742187453023	6.4505313800336292	9.9762366574871137
Ar	8.5561629487759134	19.630435410265058	11.560260061630299
Ar	16.617832469394298	8.0353659885038535	2.5675410389956719
Ar	6.3552521800231982	6.4477519078086587	10.681776949928434
Ar	2.2566824506815699	6.4599469338277018	15.841069079614973
Ar	0.54857598672281815	3.0400856403137602	9.4038973121965892
Ar	11.487623147961484	14.014856670758324	9.7474779900788668
Ar	17.298418199658773	11.976191836664691	14.352837298194657
Ar	17.550829978626467	13.007068110357993	7.3754227048444116
Ar	0.45586673776840392	13.863355849749576	4.0786902352451397
Ar	11.911030172244782	13.155277689957549	3.0151760343111742
Ar	14.215422493171983	2.0347273179991032	4.9859967392477094
Ar	2.1990768260363400	16.939458383001718	10.095514275440427
Ar	16.136287427198187	4.7546613042448307	16.578559572957747

Ar	6.5159292833833318	10.830334821278919	19.386737379461948
Ar	0.60775623660441547	9.9932598533247532	9.8726450151568059
Ar	5.5468160076857531	0.10669049546937058	13.151015934658368
Ar	4.8739589068179772	17.801316078938630	17.199426295997444
Ar	11.471484449602379	8.9472289746848119	13.815458040066886
Ar	9.3413261735416526	6.7066976999828380	1.3979069681422251
Ar	11.867388148008130	2.5556641908604716	11.527179672684449
Ar	6.0859964648166001	12.500771251358669	13.028046401176397
Ar	13.686112470782788	19.244991732362962	5.9022622882723157
Ar	11.757308817570397	7.9592905659332605	7.3988491166268000
Ar	13.354809037145875	9.8231420306819910	20.346151204055992
Ar	5.7358801758709550	12.479742328039112	-0.14445142725230342
Ar	6.9144926414367838	17.862281780037581	4.9292337743747332
Ar	6.3753131603075337	11.514331221601372	6.6102272773206394
Ar	-1.36892234065324921E-002	13.054462524461263	16.102781691526815
Ar	15.911056579755368	18.530107512471059	12.395691436582281
Ar	7.3256932007273248	1.8310601134743540	6.0827848690248754
Ar	11.302392566229889	15.217789127099143	16.439832591636723
Ar	8.7388673142050521	4.3572821584086867	17.672542332745355
Ar	2.7421576523135314	6.7320756223898046	3.9019028645149239
Li	8.9222590299431914	10.230591831047558	10.213579380048829

Structure corresponding to the blue curve:

35

E=-0.14290411470624309

Ar	4.4155991126277838	7.9240926986228137	-2.1657985705174436
Ar	7.6607933299488389	10.676535410327944	14.991442757390910
Ar	-4.5695556683984604	17.633244392152587	8.4236742265538336

Ar	3.8104483430729608	9.8845029050606517	4.6258878556470817
Ar	1.7421780946306509	13.076407571923523	17.639049625515611
Ar	-0.20841438959672676	5.5786987941629649	8.3614667809200771
Ar	6.9852178538299574	16.441973391304835	10.270311656102416
Ar	11.751422602008923	4.4166550688605515	6.3556505177882956
Ar	12.932335441294093	17.186004700661897	6.6592733179117065
Ar	5.1079945234281876	22.945191606086663	12.675499551340383
Ar	0.80525701348339540	17.674811526145525	12.732444116763707
Ar	3.4274905600667029	19.886944307047589	0.71296155579438236
Ar	7.2543601775751441	17.487830071598413	16.833797314313792
Ar	9.8497588305511528	9.0248496426822911	1.7510483237611414
Ar	13.169737371721617	7.2347919171200550	12.481080729790976
Ar	-2.7207458682122523	11.425722467008210	5.9601925160799611
Ar	6.2304988575858484	5.3917680267826436	10.472515156628589
Ar	-3.5178867557777305	11.943185643656156	12.888774709160597
Ar	9.1163900792208121	10.834003848175449	8.2412049614588749
Ar	10.434807720702628	20.261601095252125	0.12026002370226831
Ar	7.3084521921679748	21.550962180735251	6.1718111201448096
Ar	2.7857493523368912	11.482121240335415	10.668667023639653
Ar	13.858676640290280	14.302229644577817	0.39333701118882974
Ar	7.5189152029715274	15.111329521993127	3.6396366208306659
Ar	15.475391761235114	10.613390548100433	6.3104767375695507
Ar	0.50041822095824284	22.639977063348887	7.3635296840557087
Ar	-1.2070312162060619	6.3668081891444936	1.4581266653582634
Ar	1.8591550470750873	16.172629448489609	6.2520662886743272
Ar	1.2161667772734539	6.6291038867651935	15.194821362351702
Ar	11.704221671012171	21.101728211266913	12.234436256005235

Ar	7.3074541804973316	14.335415610145610	-2.9325241584496293
Ar	13.064189235317391	14.244705182659334	12.821668704355179
Ar	5.2564678903996880	3.4896846947466122	3.6420236931993788
Ar	0.83020959932202265	13.543779567179911	2.83940081855290488E-002
Li	5.3447101323324224	13.320324323529073	7.2976572010617113

Li⁺Ar₃₈ cluster of PES I

Structure corresponding to the green curve:

39

Energy=-0.11883722464559590

Ar	10.414382424260964	6.2205065483316329	6.6694434918246692
Ar	9.0348690224257986	12.737622641974184	4.4719133900966286
Ar	16.901738269246355	4.5693103145843770	9.0654602653027361
Ar	5.0160371426525758	6.6145648023554786	11.131012482107286
Ar	11.438224628841798	4.9068814720487737	13.529818034311843
Ar	15.508221950923398	11.108405500425954	6.7866293323855409
Ar	10.154298144403093	11.554138929953892	11.415928472165556
Ar	15.813551222308957	20.428379665717792	22.994469454336990
Ar	14.137175592301187	17.687399723894202	4.6203473730322209
Ar	16.418056137734450	9.9527015629195876	13.724308537062413
Ar	21.931098884012368	9.4558919339953107	9.2139172058085634
Ar	13.789995730505089	22.951331121056882	9.2433481933874084
Ar	8.6748529946929018	18.083465811093156	9.0768430213464875
Ar	15.081068537144969	16.330782302226059	11.566967304267335
Ar	11.139723264219693	10.325544905959296	18.096969558162307
Ar	17.898973419847916	3.3124227748708495	15.893712251678203
Ar	5.6783338077452230	10.594123703804922	22.681017504505562

Ar	6.0311794728769375	5.3360119779572894	18.050894293647698
Ar	20.540040614137649	16.062101298270580	6.9805533494888090
Ar	22.933871912306870	8.1948803909841157	16.041227884588267
Ar	21.616744804774488	14.777329112442178	13.843750771089969
Ar	12.428444131709455	3.7026223189758505	20.418926758942650
Ar	3.6419901678084399	13.133981346438638	8.9393315561753877
Ar	4.6049688312942045	11.882648919547158	15.820334833499551
Ar	17.543340958367050	8.5721728418189418	20.590161168929075
Ar	3.2868616536455346	18.467322871294897	13.628301916287480
Ar	20.189855076107619	21.321768792973096	11.607360440151268
Ar	22.572141343010415	13.528558946210019	20.728831587268225
Ar	9.8041359169799271	16.704348646845840	15.941277958284488
Ar	12.077547306703460	8.9632152155551079	25.044283127158238
Ar	10.713461243314319	15.544826623011597	22.879594433240950
Ar	21.208605366155346	20.047549955983250	18.528081220831467
Ar	14.786332614500298	21.749751810286369	16.132921100590288
Ar	8.3252838944363035	23.345010016131699	13.774692619286679
Ar	16.067219769920836	15.102877793282511	18.249184333226339
Ar	4.2932318294646228	17.203131258266730	20.453762016352265
Ar	9.3273416452635782	22.085862851151365	20.602776191315701
Ar	17.180795432842395	13.911437293143845	25.198930444136849
Li	13.111029870570363	13.328470948387663	14.832544106210669

Structure corresponding to the blue curve:

39

Energy=-0.11841353094957743

Ar	11.431504586449194	17.648910032800934	23.136967737897464
Ar	7.0240725087441547	18.961154374425323	18.117462109662071

Ar	11.933988519001502	20.409796074749856	29.899108085176632
Ar	9.4027699124660167	29.312913565286607	22.278093534583178
Ar	-3.6849450495106515	19.423702469690994	27.277168492061566
Ar	5.9967211162417078	22.474656103840147	12.298311077679255
Ar	0.59476616374814895	13.154240683031551	18.137304697151166
Ar	1.9327678654978360	18.860183056496137	22.487960543919147
Ar	8.0772333138013774	15.029267790488156	33.723903286721139
Ar	1.1389222784808963	16.309694820181601	31.741004294945583
Ar	5.5396859084541914	10.629768121170697	28.580438394295012
Ar	-2.0767571909663829	24.237273166474171	21.932807122181902
Ar	6.1106696712035822	13.526674174345327	22.114443583165535
Ar	16.229411282728247	12.567141262498533	22.360408601863320
Ar	2.4329248537845429	28.232290336754634	32.250285833855784
Ar	17.579684634212235	18.272737762495428	26.148857899816168
Ar	16.297716837324685	19.140738399459270	18.771710129471664
Ar	2.8681596532909137	7.5010534743710480	22.775177444662585
Ar	-1.5970240160069773	22.479174103827944	33.797611225406953
Ar	-4.4898217976723673	17.450731293887340	20.576724547089551
Ar	7.3179864934644829	22.928942044433267	23.613575996809548
Ar	5.4642039462498353	14.980606720132300	12.952077032958432
Ar	8.5354316543785842	26.683722321089103	29.064546273677980
Ar	14.110856127827910	24.154629436604356	24.147302420020932
Ar	2.1425510043451372	22.802569814272360	28.025275502865135
Ar	6.2954854875611890	17.436638088251229	27.565266876376946
Ar	3.9909414247258859	25.623045921901213	18.344792180724387
Ar	5.8273728496970110	21.687624629763917	33.603646025753577
Ar	11.893722031147956	18.814725556708652	13.045601942078449

Ar	-3.4474265188007696	26.809924626875162	28.359425614515278
Ar	11.211749436370615	24.306183360987845	17.596173706904310
Ar	-0.40532710508576825	13.215091068788007	25.445108999663109
Ar	10.348439246405466	8.4121930385922141	23.032698511066720
Ar	6.2121621904605790	8.9100410596539650	16.811686153844363
Ar	11.416376427952558	13.460712198796060	17.438950086087129
Ar	2.8717653219359520	28.724780231785996	24.810168126075901
Ar	0.36526050476305394	19.933353841903745	15.829507033847621
Ar	12.212609650428741	13.224933503057061	28.255711063829015
Li	6.6740793642671177	18.237976571861669	22.852046779248511

Structure corresponding to the yellow curve:

39

Energy=-0.11786416390033086

Ar	16.489756215546908	6.2421490200337031	4.6533167001377329
Ar	6.2249184578062824	5.2886857184787335	10.794086062481171
Ar	15.067347505361468	12.650101235279143	2.0239992836367020
Ar	9.4881540277650807	5.5165650058682747	17.395655810923358
Ar	20.410649558984428	6.8821109035888091	10.542993751301225
Ar	9.7991266225574982	8.7665023391519004	5.7295879200881235
Ar	9.9775313766145075	10.588583762327298	12.978417078462618
Ar	9.3459182316603950	22.218249263182852	14.789365842816567
Ar	-0.30005531232914828	15.525507408887856	13.141471559593271
Ar	15.156978267872482	11.631439764761305	8.7816983222628178
Ar	21.638678708580468	13.387875815101182	7.5605880743180904
Ar	4.9114916317547292	19.543231657983437	9.6179240870222333
Ar	4.6941878583213992	12.447385668081216	9.0711719673157774
Ar	11.429149293176080	16.928706962248032	11.014309917077817

Ar	16.429955788219289	9.8862003068985285	15.210705683052968
Ar	23.211314695498395	12.210449327356029	14.578620844356035
Ar	16.346623802382481	3.4060511703166600	17.331741705121047
Ar	13.421765983345892	4.9352537241646921	10.970511274888457
Ar	9.3332928187849369	15.941960876343616	4.6861826319490412
Ar	22.300417706878314	20.166903777067798	9.6662087014385687
Ar	16.333286518465759	18.238642252630196	6.2929377051179181
Ar	21.080854273815806	8.0120567582398223	20.010360328985445
Ar	3.4037606087446468	9.5476045520273161	15.642784562553461
Ar	7.9703202148039178	19.011804225369882	21.028480969151779
Ar	18.993838496527882	11.459536100791858	26.055416955932625
Ar	1.5264537696413687	15.232424795591571	20.168779595088807
Ar	10.788328437073602	22.693593763138800	7.3783229400095580
Ar	19.031401728081963	14.791750051098116	19.897273047041224
Ar	12.600804801237045	14.982640469487118	17.410410740942798
Ar	14.162369600362569	9.0771232238905171	21.558337945196584
Ar	13.348864173840870	15.627997517436320	24.183527738366898
Ar	21.577521400144544	20.620106292104282	16.681324719576633
Ar	15.984459495570395	22.671295940376353	12.234132853341830
Ar	6.2122322394669514	15.797714449560486	15.217027522465864
Ar	17.807369992635710	16.167923873417266	13.075693578292912
Ar	7.6804282646041289	11.729134603694268	20.885912902199227
Ar	2.4687307958102394	21.386362268076212	16.448149848480355
Ar	14.952788951056689	21.021504312652720	19.265756925488603
Li	13.893107089248597	13.368651402072285	13.081963739906273

Li⁺Ar₃₈ cluster of PES II

Structure corresponding to the green curve:

39

Energy=-0.15412660598152700

Ar	5.3731844116769869	9.3224960450306380	1.03369033098374020E-002
Ar	5.4745353472164551	3.0129782863587513	2.8355231731807247
Ar	5.7155636196776767	7.1825005930014605	20.698690787283159
Ar	-0.22429366945105561	16.542817308912348	7.8309843162561137
Ar	5.7661964189663939	8.0343431132001442	13.633712493155153
Ar	11.244398186482899	0.70539698103647752	6.0033903153439931
Ar	-0.22996649628741092	10.889826526776829	3.7450413066380204
Ar	11.034966019209477	13.383994137272346	0.33805310221694956
Ar	11.038014487604819	18.985532815750311	4.3900406893880861
Ar	11.056522423646943	7.1187673937883478	3.3419000027850863
Ar	5.4675815912752581	14.837242633199480	4.2328732522088313
Ar	-0.12586850879299152	4.5821820666755588	6.5736714705342321
Ar	5.3863218887782498	20.569613616062149	8.1584388142649082
Ar	10.986730857182190	12.533268870092282	7.4049689815666921
Ar	8.84486570424527219E-002	10.202099784025847	10.651286763947997
Ar	11.367726893257009	-3.32442429243675220E-003	12.879321958316373
Ar	-0.10347960980831329	15.840344681200479	14.707576145370147
Ar	16.856886345602099	4.7286715458266535	6.3300392137146995
Ar	5.6643217427977746	14.029401945854183	10.951596105070887
Ar	-3.98121719683681985E-003	3.8698814604120293	13.511067299230984
Ar	5.6786000811836086	2.4824660534524381	9.7604892971078066
Ar	16.751826771810265	11.093537329167317	3.4795098240489200
Ar	16.757982451622627	16.697615058754810	7.5276902786068431

Ar	11.088613229179165	6.5381266485338276	10.087039655149800
Ar	11.075852375343272	18.084756951259543	11.278345759335032
Ar	11.284614817874408	5.7290312113515567	16.805433635901533
Ar	5.5100091411006353	19.862958225350205	15.034900089736107
Ar	5.6555006280734901	8.7081326407575830	7.1007199743682374
Ar	11.097415326543750	11.859327193869317	13.937841716382380
Ar	16.976989844798428	4.0248280937343459	13.206998102529873
Ar	-6.28418194228456180E-004	9.4750299636534940	17.558360514554163
Ar	16.664610625371090	10.365806530432893	10.387460703929932
Ar	16.981089477820241	9.6773113514502480	17.294689754019647
Ar	5.7158160328081822	1.5799081790761751	16.647739885896993
Ar	11.279175651250206	17.552858223655157	18.203336049560995
Ar	11.376762991594362	11.243616577669982	21.028669897892325
Ar	16.879984813435676	15.984671278341846	14.465325149133598
Ar	5.6950621873862257	13.449159921431578	17.696340172833771
Li	8.3764530147284333	10.283749610548607	10.519312447606717

Structure corresponding to the blue curve:

39

Energy=-0.15353950827214846

Ar	5.4772815662200616	1.2909119466706223	3.7549886816017684
Ar	9.4052711508650297	4.7672093412610579	-1.5421549146057625
Ar	17.174802653895721	17.908465211827366	14.633780943549260
Ar	3.4879603656705038	11.754149540679860	8.4972345337389132
Ar	10.471320678874799	9.2339402551089247	9.1014423749638240
Ar	17.795750821737766	1.4889839674959038	5.4688632250058609
Ar	2.6979827858816354	5.8162603642580573	-1.2733912180530131
Ar	6.4113954732895717	10.762784103466030	-4.8096322113337511

Ar	7.4333575640756377	17.207926221707993	-0.79921308635230315
Ar	12.165346594465888	-0.37006371341139421	1.9413399930695814
Ar	3.1469849030672927	12.288789701061354	1.3117229265277459
Ar	0.33990915291232315	6.4994797108729454	5.1750240654376451
Ar	3.1585958604803008	18.278340874095271	4.8443118769493019
Ar	10.834808022498059	11.175541046158507	0.10413093612946420
Ar	7.1829044943603435	11.482563001070059	14.422996721395027
Ar	16.410624750658663	6.6438662095991923	9.9490091028727150
Ar	6.0504460379961253	17.780720478523651	11.151278368905178
Ar	16.836113903079379	4.1369926958379226	-1.4283942151320501
Ar	8.5956760119946409	14.157017186767682	5.2062773645503180
Ar	5.0214907882041979	5.2775594917102921	10.277702050496949
Ar	10.877108328956098	2.3436410718621046	8.2488180146182142
Ar	12.438376306459897	15.117279439233702	-5.2752673709136531
Ar	13.202702768971633	8.2915895148254837	-5.9362735620261216
Ar	13.337100825877195	6.4003138661006140	3.7209579165840667
Ar	9.9401101297372740	20.648912734703089	5.6894155676444935
Ar	14.430238940115069	11.054591029678228	15.101240683931147
Ar	11.955725705186888	22.070641385065183	12.197529465991520
Ar	6.9919304225259351	7.7326828217492665	4.0441434589838279
Ar	14.879434340849835	12.307121232552786	5.3526825747832101
Ar	20.104078019391014	8.0279906799381084	4.2987688372420028
Ar	10.530269652769432	17.020048823294836	16.988597047871643
Ar	17.285535236144927	11.215458363631374	-1.0801229499595133
Ar	20.823381527001668	15.104156127824547	3.4723780558940560
Ar	10.732251526284003	5.1834477248938562	14.596103104933794
Ar	16.769195554690555	19.182606240907020	7.3845316848256175

Ar	19.348644716513551	12.978862986434432	10.226561921846725
Ar	14.038323492781377	17.249739526166479	1.1624013586435886
Ar	12.256391301401097	15.408033637737958	10.534056304656811
Li	10.857927901120588	10.191570404282681	4.6153009007972656

Structure corresponding to the yellow curve:

39

Energy=-0.15294429816172550

Ar	-2.0409878915787139	8.3285233805723973	10.229861846828744
Ar	11.290371591493262	3.3630934970738435	20.351866477790640
Ar	9.4724535209608973	14.835959386186676	15.524520274626720
Ar	9.6826185560050426	9.4594774139353781	2.6206333310031265
Ar	9.2628598069541273	8.7946379427535248	12.458034387126308
Ar	1.1052266748278279	2.5118816146896874	7.1825984961837976
Ar	-0.62237586117638699	7.8245253333568554	17.551883164356852
Ar	11.941295142112303	2.6928754089206355	2.9133500390855169
Ar	9.6157440908537382	13.863776011736011	8.1823167486551398
Ar	7.0897801608879805	-1.9602914076614091	5.5835828807964578
Ar	5.1059316606086274	4.2514740797432147	1.7945688826673372
Ar	8.4670272464282128	-3.1230415972611270	18.005110630740877
Ar	16.834548891111886	7.5051880543043907	1.7637010347631135
Ar	13.401772188211400	1.1579622150050506	9.4194807183771925
Ar	3.5583125927426007	5.5542403651416992	12.766861308425190
Ar	20.357950748515872	9.1984369182744494	15.635855663344469
Ar	4.2800533838200279	9.5850592504096568	7.1308198194598518
Ar	14.772866663361107	-0.91279424210635163	15.792958839651050
Ar	13.378704741854447	7.4093950334026104	7.6825765109920940
Ar	6.5395109172683625	8.2077672402283586	18.487023453941617

Ar	-2.0104052480466179	1.8365668343816839	13.711177182911154
Ar	13.776698360161710	-3.7777574162685399	4.6835407171619394
Ar	4.1758709958070845	-1.3802277380071024	12.019558405125530
Ar	9.1628718591724425	2.4522945431604044	14.185778891687526
Ar	-1.0488700770392478	7.7321254341790082	3.0869053158114297
Ar	15.133527634010422	12.243200720195542	12.194505335734103
Ar	3.2883314340601864	12.337606905168046	13.454269478900102
Ar	7.8205098496840737	4.1075385873492634	8.0182941035627238
Ar	14.787316887644691	5.6638569448914593	13.812107977691770
Ar	17.768567053454113	-4.0511470000950540	10.312217376948613
Ar	3.6181865378118445	1.8603568098492804	18.477739861412104
Ar	20.199002823954526	2.1337117790220947	12.428768103156330
Ar	18.629837619025640	1.8900802505441547	5.4902587032044483
Ar	10.423278671956869	-4.3846469827489329	11.372718030332241
Ar	15.948841346991316	13.333037402734830	5.3435485455550946
Ar	18.191249785530676	3.8995012542179812	19.482281348422756
Ar	13.365515967623901	9.9001304752960557	18.649923923597580
Ar	19.835240865965392	8.0687694959292227	8.7562058474371067
Li	11.256182849179300	4.9432717668263351	10.943917107600017