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Supporting Information

Are phosphide nano-cages better than nitride nano-cages? A kinetic, thermodynamic and non-linear optical properties study of alkali metal encapsulated $X_{12}Y_{12}$ nano-cages

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Table SI-1. Comparison of β_0 calculated through two level model and its comparison with hyperpolarizability values obtained at CAM-B3LYP method.

	α	B_0	ΔE	Δμ	f_0	Δμ. f_0/ ΔE^3 (β_0 from two level method)	CT
Li@AlN	571.15	453.30	1.3829	0.1526	0.1349	156.8122	H-L+1
Na@AlN	577.79	35.60	1.3914	0.0731	0.1389	75.93627	H-L
K@AlN	618.64	49.34	1.3283	0.1470	0.1186	149.8646	H-L
Li@AlP	662.30	2922.45	1.320	2.3077	0.0271	547.7879	H-L+2
Na@AlP	681.46	448.08	1.506	0.3024	0.0355	63.31708	H-L+2
K@AlP	741.57	115.90	1.5887	0.3643	0.0431	78.88535	H-L+5
Li@BN	173.30	395.46	2.3754	2.1963	0.0202	66.6835	H-L
Na@BN	177.52	100.21	1.9867	2.8438	0.026	189.9596	H-L+2
K@BN	188.27	120.22	1.7919	3.1126	0.0217	236.4979	H-L+2
Li@BP	376.93	15582.64	1.2807	1.7590	0.0289	487.5364	H-L+2
Na@BP	501.64	336.26	1.4312	1.5449	0.0336	356.7174	H-L+5
K@BP	989.79	564230.9	0.7645	0.0514	0.0077	17.84461	H-L+5

Table SI-2. Vibrational analysis of alkali metal encapsulated AlN nano-cages

AlN		Li@AlN		Na@AlN		K@AlN	
Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity
933	674	910	23	899	21	877	11
895	330	865	123	853	126	829	113
684	236	672	44	663	56	649	67
	119	656	39	640	25	628	8
532	44	565	150	497	163	490	184
401	155	-	-	-	-	-	-
318	-	-	-	305	7	312	7
-	-	80	46	160	8	-	-
-	-	42	45	-	-	-	-

Table SI-3. Vibrational analysis of alkali metal encapsulated AlP nano-cages

AlP		Li@AlP		Na@AlP		K@AlP	
Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity
530	313	538	15	512	170	495	173
500	36	515	139	489	31	475	2
460	34	496	48	451	26	440	16
		460	35	-	-	-	-
340	4	-	-	-	-	330	9
222	7	201	14	217	19	267	8
-	-	147	16	56	32	-	-
-	-	126	16	50	32	-	-
-	-	106	6	36	30	-	-

Table SI-4. Vibrational analysis of alkali metal encapsulated BN nano-cages

BN		Li@BN		Na@BN		K@BN	
Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity
1424	1363	1440	194	1408	187	1311	151
		1413	420	1373	303	1284	276
		1404	1155	1369	1134	1271	1074
		1384	966	1341	890	1244	787
		1347	552	1304	485	1210	416
1203	85	1272	20	1233	22	1169	38
		1229	40	1186	47	1140	16
						1068	131
808	248	838	141	846	91	866	170
806	246	804	168	838	115	856	170
				822	127	833	31
				799	30	764	25
						752	32

Table SI-5. Vibrational analysis of alkali metal encapsulated BP nano-cages

BP		Li@BP		Na@BP		K@BP	
Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity	Wavenumber (Cm^{-1})	Intensity
894	193	870	56	860	90	834	86
761	22	746	14	736	14	707	10
		408	24	465	11	491	5
		456	5	421	13	425	6
		340	26	337	22	333	22
		111	41	187	7	203	3
		87	40	181	6		
		48	39	179	6		

The D3 problem of Gaussian 09 for endohedral fullerenes

D3 correction of any method is not possible for endohedral fullerenes in Gaussian 09. Optimization of EMFs fails because of the problem in Gaussian 09 code. A recent communication with Gaussian Inc is also copied.

Hello Khurshid

There is a known problem with some terms in the second derivatives of the D3 dispersion model. In the D3 expressions, there is one term that depend on the “coordination number” of the atoms involved (the "coordination numbers” are determined on-the-fly according to rules given in the model). The analytic expression for the second derivative of such term is not numerically stable for large coordination numbers (~8 or higher), which is going to lead to NaNs (Not-A-Number) in the contributions from D3 to the energy second derivatives. The structures where you find these problems must have one or more centers for which the coordination number is ~8 or higher. Unfortunately then, in such cases, there is no way around this issue in G09 rev. D.01. We have worked out alternative expressions for the D3 second derivatives that can avoid this numerical instability and we hope to have this available in a future release of Gaussian.

Even though the optimization with d3 correction is not possible, attempt has been made to optimize all geometries with B3LYP-D3 and only a few EMFs are successfully optimized, mostly lithium encapsulated ones. The optimization of Li-EMFs is sensible because the lithium atom in some fullerenes is not present at the center rather it is present towards one side where the coordination number of lithium is less than 8. (the purpose of optimization of these EMFs with D3 correction was to get some idea about the thermochemistry and electronic properties)

Table SI-6 Comparison of thermochemistry with wB97XD, B3LYP and B3LYP-D3 using 6-31G(d,p) basis set.

	ωB97XD			B3LYP			B3LYP-D3
	E_{bind} (Kcal mol^{-1})	E_{BC} (Kcal mol^{-1})	E_{dist} (Kcal mol^{-1})	E_{bind} (Kcal mol^{-1})	E_{BC} (Kcal mol^{-1})	E_{dist} (Kcal mol^{-1})	
Li@AlN	-2.78	111	6.22	-2.92	97	8.98	-15.23
Na@AlN	22.56	263	14.4	22.62	247	15.71	
K@AlN	71.72	567	30.5	69.02	518	30.94	
Li@AlP	-26.06	31	10.1	-13.6	20.1	9.66	-29.41
Na@AlP	-12.88	140	0.1	1.6	127.3	0.77	-17.35
K@AlP	17.54	323	12.1	19.71	278.5	17.81	
Li@BN	48.99	216	48.4	52.08	191	44.33	
Na@BN	115.66	697	56.3	119.09	615	51.95	
K@BN	267.5	1315	85.2	273.58	1109	81.71	
Li@BP	-24.54	85	0.6	-21.43	73	0.87	-37.14
Na@BP	-3.91	262	17.9	-2.84	255	3.08	
K@BP	38.80	584	17.5	39.27	492	13.09	

The B3LYP-D3 results show that the formation of these EMFs is more favorable than with B3LYP method (more exothermic or less endothermic). Large differences in binding energies calculated at B3LYP and B3LYP-D3 methods were forcing enough to perform all thermochemistry with some dispersion corrected method. ωB97XD method is a better method for coordination chemistry of alkali metals, as revealed from a benchmark study by Carlo Adamo and co-workers[1]. The Study by Adamo reveals that ωB97XD is good method not only for interaction energies but also for potential energy surface. The latter is very useful point related to this study because PES surfaces are also scanned for translation of alkali metal into the nano-cage.

A comparison of interaction energies at B3LYP, B3LYP-D3 and ωB97XD is given in the table above. The binding energies at B3LYP-D3 are the highest among all whereas those with B3LYP are the lowest. B3LYP-D3 method is known in the literature by our group[2] and others[3,4] to overestimate the binding energies. As the literature reveals that ωB97XD provides better results for thermochemistry of alkali metal coordination chemistry, the results with ωB97XD are now incorporated in the manuscript.

Although the binding energies are more favorable with dispersion corrected methods; however, the barriers for boundary crossing are increased. B3LYP method underestimated the boundary crossing barriers. Despite the fact that the values are changed with ωB97XD however the trends and important findings remain unaltered.

Electronic properties

The choice of B3LYP method is mainly due to the validity of B3LYP method for electronic properties, not only for these inorganic fullerenes but also for conducting polymers[2,5–8] and other systems[9]. Other functional are generally poor in this regard. A short benchmarking is carried out against experimental data.

The band gap for AlN, AlP, BN and BP are taken from the literature, and appropriate references are given. It is worth mentioning that band gaps for Al12N12, Al12P12, B12N12 and B12P12 could not be retrieved from the literature. However, the values for other related forms are taken from the literature. For example, band gaps for hexagonal BN, Cubic BN or BN nano-tubes are considered and all of them lie in the range of 5.5 to 6.5 eV. It is expected that the band gap for B12N12 will lie in the same range or a bit higher.

These materials are semi-conductors and their band gaps are expected in the range of 1.5-6.5 eV. The theoretical values for the band gaps are compared with the experimental data. Except for AlN, the calculated band gaps are overestimated by about 1 eV with B3LYP and B3LYP-D3 methods. The band gap for Aluminum nitride is slightly underestimated with these functionals. Although the band gaps calculated with these functionals are not the perfect match with the experiment (which could be due to slightly different nature of the material taken as reference) however, these are the closest values. A number of strides have been made in the literature in this regard but no other functional is consistently better than B3LYP for the band gaps.

The band gaps calculated with M05-2X deviate from experiment up to 5 eV whereas this number reaches to about 6 eV with ωB97XD. The band gaps calculated with these functional suggest that these materials should be insulators which is not the case.

Table SI-7 Comparison of band gaps of (XY)n semiconductors calculated with different functionals with experimental values.

Nano-cage	Exp	B3LYP	B3LYP-D3	M05-2X	ωB97XD
AlN[10]	5.11	3.93	3.98	8.22	9.09
AlP[11]	2.45	3.39	3.37	7.87	7.63
BN[12]	5.96-6.36	6.85	6.86	9.49	10.58
BP[13]	2.4	3.70	3.74	8.08	8.38

Now comparing band gaps at B3LYP (on B3LYP optimized geometry) with B3LYP-D3 (on B3LYP-D3 optimized geometries) method, one can see that the former is a better match with the experiment (although the difference is negligible). Because of this fact, the discussion on electronic properties is not changed in the resubmitted manuscript. The band gap (and related discussion) is retained at B3LYP/6-31G(d,P) on B3LYP/6-31G(d,p) optimized geometries.

As far as NLO properties are concerned, the literature reveals that the hyperpolarizability values calculated at CAM-B3LYP correlate better with those from coupled cluster calculations. A few other better methods are LC-BLYP, M05-2X, M11L and ωB97XD; however the reports in favor of CAM-B3LYP are more than for other methods. Due to this fact, CAM-B3LYP method was used. These important references for CAM-B3LYP are now added into the manuscript.

Since geometries of EMFs are also optimized with ωB97XD and B3LYP-D3 (a few of them), hyperpolarizabilities are calculated on all these geometries to see if any big difference could be observed. The hyperpolarizability values at CAM-B3LYP for all these structures are compared in the table below. As one can see that the individual values are changed slightly however the trends are similar. These differences do not influence the results presented in original submission therefore, the original values reported in the first submission are retained whereas the other values are given in the supporting information. And necessary text is added in the manuscript for these values.

Most of the discussion above is also provided in the supporting information for readers.

Table SI-8 calculated electronic properties of alkali metal encapsulated nano-cages. (Bold values are on B3LYP optimized geometries whereas bold and bold italic values are based on ωB97XD and B3LYP-D3 optimized geometries, respectively)

Nano-cage	E_H (eV)	E_L (eV)	ΔE_{HL} (eV)	%_HLG	E_{FL} (eV)	A (au)	β_o (au)
Li@AlN	**-3.55**	**-1.69**	**1.86**	**47.3**	**-2.62**	**571.15**	**453.30**
	-3.51	*-1.64*	*1.87*	*46.4*	*2.57*	*556.9*	*720.9*
	-3.52*	***-1.69***	***1.83***	***46.0***	***-2.58***	***571.54***	***532***
Na@AlN	**-3.55**	**-1.7**	**1.85**	**47.1**	**-2.63**	**577.79**	**35.60**
	-3.50	*-1.64*	*1.86*	*46.1*	*-2.57*	*571.1*	*25.2*
K@AlN	**-3.53**	**-1.75**	**1.78**	**45.3**	**-2.64**	**618.64**	**49.34**
	-3.47	*-1.70*	*1.78*	*43.9*	*-2.58*	*622.3*	*8.4*

Li@AlP	**-4.73**	**-2.97**	**1.76**	**51.9**	**-3.85**	**662.30**	**2922.45**
	-4.89	*-2.83*	*2.06*	*60.1*	*-3.86*	*647.9*	*3337.5*
	-4.86*	***-2.85***	***2.01***	***59.6***	***-3.86***	***653.7***	***3662.0***
Na@AlP	**-4.58**	**-2.8**	**1.78**	**52.5**	**-3.69**	**681.46**	**448.08**
	-4.62	*-2.66*	*1.96*	*57.1*	*-3.64*	*668*	*720.6*
	4.62*	***2.70***	***1.92***	***57.0***	***-3.66***	***671.57***	***530.8***
K@AlP	**-4.23**	**-2.49**	**1.74**	**51.3**	**-3.36**	**741.57**	**115.90**
	-4.08	*-2.4*	*1.68*	*49.0*	*-3.24*	*725.2*	*170.8*
Li@BN	**-4.02**	**-1.38**	**2.64**	**38.5**	**-2.7**	**173.30**	**395.46**
	-4.06	*-1.33*	*2.73*	*39.3*	*-2.69*	*171.6*	*425.7*
Na@BN	**-3.84**	**-1.59**	**2.25**	**32.8**	**-2.72**	**177.52**	**100.21**
	-3.92	*-1.53*	*2.39*	*34.3*	*-2.72*	*175.1*	*181.8*
K@BN	**-3.97**	**-1.92**	**2.05**	**29.9**	**-2.95**	**188.27**	**120.22**
	-4.04	*-1.86*	*2.18*	*31.3*	*-2.95*	*185.5*	*87.9*
Li@BP	**-4.19**	**-2.69**	**1.5**	**40.5**	**-3.44**	**376.93**	**15582.64**
	-4.18	*-2.67*	*1.51*	*40.5*	*-3.42*	*374.6*	*11540.8*
	*-4.15**	*-2.67*	*1.48*	*39.5*	*-3.41*	*370.5*	*10445*
Na@BP	**-4.14**	**-2.77**	**1.37**	**37**	**-3.46**	**501.64**	**336.26**
	-4.15	*-3.25*	*0.9*	*24.2*	*-3.70*	*421*	*1214*
K@BP	**-3.66**	**-3.26**	**0.40**	**10.8**	**-3.48**	**989.79**	**564230.9**
	-3.92	*-3.15*	*0.78*	*20.8*	*-3.54*	*410.2*	*4614.6*

* Band gaps are calculated at B3LYP-D3/6-31G(d,p)

Notes and References

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Note: To obtain barriers for boundary crossing, initial geometries are those obtained at B3LYP/6-31G(d,p)

Table SI-9 Total, ZP and Gibbs energies of optimized geometries at B3LYP/6-31G(d,p)

File Name	SCF Energy (A.U)	SCF Energy (Kcal)	ZP Energy (A.U)	ZP Energy (Kcal)	Gibbs Free E (A.U)	Gibbs Free E (Kcal)
Li@AlN	-3574.739182	-2243182.797	-3574.66287	-2243134.91	-3574.713032	-2243166.387
Na@AlN	-3729.487371	-2340288.755	-3729.410868	-2340240.749	-3729.458858	-2340270.863
K@AlN	-4167.023958	-2614847.12	-4166.947524	-2614799.157	-4166.99428	-2614828.497
Li@AlP	-7013.82778	-4401243.563	-7013.7828	-4401215.338	-7013.846373	-4401255.231
Na@AlP	-7168.59229	-4498359.764	-7168.548577	-4498332.333	-7168.614671	-4498373.808
K@AlP	-7606.174136	-4772946.529	-7606.130615	-4772919.219	-7606.195376	-4772959.857
Li@BN	-963.5534521	-604638.9449	-963.425201	-604558.4662	-963.461564	-604581.2843
Na@BN	-1118.235546	-701703.4282	-1118.108169	-701623.4981	-1118.144226	-701646.1242
K@BN	-1555.599896	-976153.7132	-1555.47633	-976076.1741	-1555.512198	-976098.6816
Li@BP	-4402.179334	-2762409.353	-4402.106129	-2762363.416	-4402.156948	-2762395.305
Na@BP	-4556.938605	-2859522.266	-4556.864637	-2859475.85	-4556.913352	-2859506.419
K@BP	-4994.482032	-3134084.923	-4994.408451	-3134038.75	-4994.456519	-3134068.913
Li	-7.490984665	-4700.664042	-7.490985	-4700.664252	-7.504387	-4709.074134
Na	-599.890422	-376436.9388	-599.890422	-376436.9388	-599.906252	-376446.8722
K	-162.2798806	-101832.1667	-162.279881	-101832.167	-162.294964	-101841.6317
AlN	-3567.243534	-2238479.207	-3567.164786	-2238429.791	-3567.209395	-2238457.784
ALP	-7006.315116	-4396529.295	-7006.270558	-4396501.335	-7006.330064	-4396538.675
BN	-956.1454622	-599990.3609	-956.016405	-599909.3763	-956.051288	-599931.2657
BP	-4394.654195	-2757687.256	-4394.579849	-2757640.604	-4394.625588	-2757669.305

Cartesian Coordinates of Optimized Geometries at B3LYP/6-31G(d,P)

Li@AlN

Al	-1.66003500	2.27101200	0.39186900
Al	-2.05812400	0.92076900	-1.72981100
Al	0.75424300	2.24308300	-1.57084300
Al	-2.61772100	-0.64184800	0.89961800
Al	-0.44775100	0.62505200	2.73342500
Al	1.24044400	2.07140800	1.49316000
Al	0.44810100	-0.62506400	-2.73515200
N	-1.96211800	-2.21955900	0.15082900
N	-2.83494900	0.88556900	-0.03375200
N	-1.53780300	-0.77578800	2.41517000
N	-1.02635600	2.42891700	-1.35506400
N	-0.58368700	2.25561700	1.83758300
N	1.96405600	2.22262200	-0.15122300
N	1.53736600	0.77597500	-2.41462300
N	-1.40689500	-0.54563300	-2.55283900
Al	1.66217900	-2.27259700	-0.39088700
Al	2.05763400	-0.92051400	1.73079800
N	1.02673900	-2.42921700	1.35603200
N	2.83313000	-0.88377100	0.03428800
N	0.58357600	-2.25367900	-1.83545300
N	1.40678300	0.54569900	2.55312000
Al	-0.75425000	-2.24307700	1.57178300
Al	2.61756300	0.64353600	-0.89931100
Li	-0.00129000	-0.01141200	-0.00560600
Al	-1.24190200	-2.07276000	-1.49554600

Na@AlN

Al	1.96358900	-1.52888800	1.41699700
Al	-0.42167100	-2.46896400	1.38789600
Al	-0.15061700	0.29634900	2.84397400
Al	0.92284900	-2.29681500	-1.43949600
Al	2.65111900	0.28992200	-1.04415200
Al	2.11443000	1.58734500	1.10103000
Al	-2.65076900	-0.29009800	1.04405500
N	-0.71278000	-1.83048900	-2.21652900
N	1.07833200	-2.74410700	0.30592500
N	1.81698800	-0.83520700	-2.18858600
N	0.50781700	-1.36726000	2.57903600
N	2.85970200	-0.09587200	0.77351800
N	0.71328900	1.83189600	2.21808600
N	-1.81638700	0.83511800	2.18807100
N	-2.04134400	-2.02664300	0.71489600
Al	-1.96347800	1.52851200	-1.41728300
Al	0.42155800	2.46883800	-1.38830100
N	-0.50791300	1.36747200	-2.57966900
N	-1.07822500	2.74366800	-0.30602900
N	-2.85987900	0.09582900	-0.77366400
N	2.04092700	2.02603300	-0.71475500
Al	0.15101300	-0.29596400	-2.84398900
Al	-0.92255300	2.29717600	1.43968300
Na	-0.00053400	0.00017300	0.00045000
Al	-2.11530400	-1.58779400	-1.10095600

K@AlN

Al	-0.90399900	-1.23285500	-2.46457800
Al	-2.38404500	-1.60967800	-0.37393600
Al	0.53341600	-2.84751400	-0.13449100
Al	-2.17445700	1.43047500	-1.28142100
Al	0.80856400	1.44401200	-2.38229600
Al	2.15897600	-0.69022500	-1.80886000
Al	-0.80875400	-1.44338500	2.38205500
N	-2.14948100	1.97067300	0.51636300
N	-2.37509500	-0.31987300	-1.73887500
N	-0.59484000	2.36570700	-1.67944600
N	-0.95749500	-2.56179900	-1.13868600
N	0.64334900	-0.36279100	-2.86753700
N	2.15041100	-1.97191400	-0.51606800
N	0.59440300	-2.36499200	1.67921900
N	-2.36621700	-1.12679200	1.38116500
Al	0.90445200	1.23264500	2.46428900
Al	2.38434700	1.60945500	0.37358700
N	0.95718500	2.56018300	1.13755400
N	2.37691600	0.32010200	1.73958600
N	-0.64304800	0.36336700	2.86853400
N	2.36572200	1.12656100	-1.38136900
Al	-0.53415800	2.84778400	0.13462900
Al	2.17390800	-1.43001600	1.28189100
K	0.00001400	0.00027600	-0.00077700
Al	-2.15924400	0.68974400	1.81003100

Li@AlP

Al	0.78758600	-1.84613700	2.42944100

Al	-1.30685700	-2.76678700	0.81070600
Al	-1.97809000	0.23951000	2.44067800
Al	1.78056500	-2.54162500	-0.77714700
Al	3.05332300	0.24785100	0.80495300
Al	1.21111600	1.59143900	2.43605300
Al	-1.36541900	-1.74518500	-2.54480500
Al	-3.09531200	-0.27045700	-0.75909200
Al	-0.84380000	2.05483900	-2.53728000
Al	1.30845300	2.81593200	-0.76523700
Al	2.18771400	-0.29439500	-2.55031000
Al	-1.73831900	2.51464600	0.82241400
P	3.67198700	-1.13481400	-0.95930600
P	1.45988300	1.86430400	-2.90429300
P	2.77249500	2.58231400	0.97234600
P	-0.91171100	2.25887900	3.00398700
P	-0.85569400	3.75209300	-0.93723600
P	-3.62102800	1.10520300	0.98702600
P	-1.49336300	-1.93550100	2.99724200
P	-2.35143300	0.34787500	-2.89675800
P	0.85566100	-3.69325700	0.96492200
P	-2.82423100	-2.61173400	-0.94436600
P	0.86680200	-2.19272700	-2.90946100
P	2.43047700	-0.34213500	2.98940900
Li	-0.00338700	-0.00089800	-0.99583800

Na@AlP

Al	-0.96673400	-0.87290800	-2.97626100
Al	1.22315300	0.97445700	-2.85133900

Al	-1.81394900	2.25162100	-1.47591300
Al	1.94589200	-2.21175600	-1.38788000
Al	-1.30720800	-2.97508600	-0.10920200
Al	-3.14752300	-0.77941700	-0.15385400
Al	3.15672900	0.78719600	0.15370700
Al	1.30174900	2.97663900	0.10828700
Al	0.96224500	0.87577500	2.98015700
Al	-1.22685300	-0.97141300	2.84793400
Al	1.81749600	-2.25982400	1.48071600
Al	-1.94220000	2.20356800	1.38362400
P	0.85242000	-3.78744500	-0.02640400
P	0.99723500	-1.42555600	3.46931900
P	-2.71296900	-2.25008500	1.63195600
P	-3.58953100	1.48485400	-0.13512100
P	-1.30807300	1.31069600	3.41536800
P	-0.85559300	3.78889800	0.02655000
P	-1.00042900	1.42700700	-3.47237300
P	2.54987100	2.18998400	1.94166400
P	1.30424900	-1.30933000	-3.41173500
P	2.70955100	2.25174900	-1.63254700
P	3.58381300	-1.48116300	0.13502900
P	-2.55456400	-2.18928800	-1.94261700
Na	0.02944800	-0.01272000	0.00126800

K@AlP

Al	-3.02057600	-0.67713800	-1.35677500
Al	-0.72362300	-2.14512200	-2.51161400
Al	-0.50547100	1.54008900	-2.96172300

Al	-1.32150800	-2.92081900	1.08573700
Al	-2.55881100	0.42169700	2.16967400
Al	-2.15839600	2.58949200	0.19636600
Al	2.16567800	-2.59499600	-0.19989900
Al	2.55714600	-0.41872300	-2.17078600
Al	3.02281000	0.68317600	1.35514400
Al	0.72231700	2.14828400	2.50623500
Al	0.50445800	-1.54256800	2.97002900
Al	1.31622500	2.91530800	-1.08180500
P	-1.84927400	-1.63450700	2.98671200
P	1.87625400	0.28852500	3.37417200
P	-1.56745900	2.53597700	2.47503200
P	-0.92813500	3.40999600	-1.59450300
P	2.35774000	2.91366600	0.99424700
P	1.84716100	1.63685700	-2.98630300
P	-1.87909400	-0.28528000	-3.37916800
P	3.76966800	-0.86997800	-0.20296100
P	-2.35617200	-2.90687700	-0.99476100
P	1.56686100	-2.53288300	-2.47736700
P	0.92687800	-3.40534000	1.59224100
P	-3.77075400	0.87365500	0.20105100
K	0.00482500	-0.01789400	0.00876500

Li@BN

N	1.88394800	-0.91996400	1.11656100
N	1.87898300	1.42944200	0.00001300
N	1.88257900	-0.91819600	-1.11977700
N	-0.13463400	2.42502100	0.00185100

N	0.46478700	1.00947900	-2.11178700
N	-1.93644500	0.91404700	-1.12123700
N	-1.93523900	0.91240800	1.12463800
N	0.46712800	1.00639200	2.11275400
N	0.07684900	-2.39919500	-0.00179000
N	-1.95724300	-1.43583600	0.00000300
N	-0.50438800	-1.01802800	2.11879700
N	-0.50671900	-1.01497000	-2.11981500
B	0.88780000	-0.44158500	1.99661300
B	0.85413800	1.81621100	0.96937500
B	-0.88946100	0.41422200	1.98969700
B	-0.87912800	-1.80342900	0.97065600
B	-1.39428800	1.74298000	0.00202000
B	-2.23205200	-0.02052800	0.00119000
B	-0.89163800	0.41712300	-1.98811700
B	-0.88015200	-1.80201600	-0.97235400
B	0.85308900	1.81764100	-0.96766000
B	0.88555900	-0.43865400	-1.99820900
B	1.38912800	-1.73589200	-0.00192100
B	2.55675600	0.04081100	-0.00148500
Li	0.31466800	0.01045900	-0.00016200

Na@BN

N	-1.86462700	-0.98515700	-1.12664400
N	-1.93548000	1.39200000	0.00076700
N	-1.86511700	-0.98726000	1.12464100
N	0.05980000	2.43063600	0.00198900
N	-0.50158800	0.99237500	2.12418200

N	1.90544000	0.97241900	1.12569400
N	1.90577000	0.97413700	-1.12332000
N	-0.50073900	0.99581600	-2.12289300
N	-0.00074700	-2.41139900	-0.00190800
N	1.99944100	-1.37541000	-0.00072300
N	0.53574900	-1.00227100	-2.12513900
N	0.53503000	-1.00555700	2.12369400
B	-0.89018100	-0.47401800	-2.01773800
B	-0.92558500	1.80853600	-0.97874300
B	0.88523200	0.45180800	-2.02507700
B	0.94406600	-1.80359700	-0.98932300
B	1.35812100	1.81899500	0.00171000
B	2.26424100	0.04894300	0.00056800
B	0.88438100	0.44870400	2.02602900
B	0.94379700	-1.80513000	0.98682000
B	-0.92611400	1.80696000	0.98134900
B	-0.89093200	-0.47730500	2.01667600
B	-1.34946900	-1.78929900	-0.00154500
B	-2.54854100	-0.03447900	-0.00062600
Na	-0.05960100	0.00610000	-0.00026200

K@BN

N	1.79914100	1.63680200	-0.00000100
N	0.40402700	1.05139800	2.15582600
N	-0.31788900	2.44106800	0.00001600
N	-0.43075000	-1.06357600	2.15351000
N	-2.01988100	0.78101300	1.13567000
N	-1.86184200	-1.59382100	0.00000400

N	0.24844100	-2.43220500	-0.00001600
N	1.98320200	-0.81392000	1.14307200
N	0.40399700	1.05142500	-2.15582100
N	-0.43078400	-1.06354700	-2.15351500
N	1.98318700	-0.81390700	-1.14311600
N	-2.01989900	0.78103300	-1.13563000
B	2.55547000	0.23513000	-0.00000800
B	0.95972900	-0.39724400	2.06375900
B	1.56465300	-1.68915600	-0.00002500
B	0.95969900	-0.39722100	-2.06377800
B	-0.76675500	-1.93232000	1.01124700
B	-0.76677400	-1.93230800	-1.01125900
B	-2.30261000	-0.18949900	0.00001600
B	-0.94353700	0.36641300	-2.06969400
B	-0.94350700	0.36638500	2.06971300
B	-1.57377300	1.70707200	0.00002200
B	0.74639700	1.94380500	-1.00439800
B	0.74641000	1.94379500	1.00441200
K	0.03349100	0.00754700	-0.00000200

Li@BP

B	0.99087300	-1.50153500	-2.05952900
B	0.57581300	-2.57273200	0.72223700
B	-1.31740400	-1.86393600	-1.50832800
B	-0.73469300	0.93189800	-2.46240200
B	-2.04262200	-1.22515200	1.34340000
B	-2.68266800	0.48650000	-0.21221900
B	-0.98842300	1.50046500	2.05755300

B	-0.57471200	2.57212000	-0.72080200
B	0.73479700	-0.92981100	2.46168800
B	1.31543700	1.86084200	1.50602900
B	2.04149500	1.22500300	-1.34145500
B	2.68108100	-0.48507100	0.21269100
P	-2.83313400	-1.43695000	-0.41545200
P	-2.63788200	0.58115100	1.72447100
P	-0.65830400	-2.25060600	2.18340000
P	0.20424700	-2.99888000	-1.10937600
P	-0.58197300	-0.89604800	-3.01990900
P	2.17639100	-1.80740800	1.50570300
P	2.63774100	-0.58083800	-1.72415700
P	2.83477800	1.43778000	0.41570900
P	0.65854000	2.25171100	-2.18320600
P	-2.17596800	1.80784700	-1.50483900
P	-0.20374600	3.00002700	1.10994900
P	0.58268000	0.89689200	3.02148100
Li	-0.01514000	-0.02104600	-0.01697400

Na@BP

B	2.70858000	-0.44244800	0.29149600
B	1.35201000	-0.08806600	-2.40198100
B	2.04628600	1.84571200	-0.16489200
B	0.96836600	0.77101100	2.46341200
B	-0.58576700	2.12688800	-1.65536600
B	-0.77346100	2.54701800	0.72341700
B	-2.70661000	0.43937800	-0.29096300
B	-1.35324000	0.08570800	2.40015900

B	-0.97025300	-0.77263200	-2.46097200
B	-2.04335400	-1.84322100	0.16448400
B	0.58255500	-2.12685400	1.65385500
B	0.77002900	-2.54674200	-0.72247000
P	0.63268400	3.10587600	-0.49848400
P	-2.19488400	2.27133300	-0.57387200
P	-0.18378700	0.89587300	-3.07569600
P	2.84688000	0.55067300	-1.37507900
P	2.61875200	1.06207600	1.52060700
P	0.62270800	-1.88598400	-2.52162400
P	2.19289300	-2.27239500	0.57388800
P	-0.63450000	-3.10807900	0.49874700
P	0.18172900	-0.89758800	3.07628500
P	-0.62484300	1.88431100	2.52161900
P	-2.84817800	-0.55236900	1.37522000
P	-2.62065400	-1.06391600	-1.52071600
Na	0.01748000	0.01582200	-0.00130300

K@BP

B	-1.09493700	2.56855700	0.32685700
B	-0.14573900	0.81299500	2.68623700
B	1.37244200	2.39927300	0.51215900
B	0.28306600	1.62737700	-2.27414200
B	2.40485800	-0.37228000	1.40699400
B	2.61550800	0.02775900	-1.03018000
B	1.09447700	-2.56886400	-0.32691900
B	0.14628500	-0.81300200	-2.68604100

B	-0.28254300	-1.62757900	2.27416500
B	-1.37291600	-2.39883700	-0.51215000
B	-2.40526300	0.37230100	-1.40699800
B	-2.61565100	-0.02756900	1.02917000
P	2.93485900	1.25702300	0.45950500
P	2.77220700	-1.64875800	-0.03088900
P	1.22436900	-0.56351400	2.92966200
P	0.03261700	2.58469400	1.92770000
P	0.28327200	3.06123700	-0.97337700
P	-1.71138700	-0.36183700	2.70820700
P	-2.77282800	1.64908600	0.03070400
P	-2.93556400	-1.25719500	-0.45977800
P	-1.22383300	0.56324000	-2.92840500
P	1.71210100	0.36192500	-2.70914300
P	-0.03280800	-2.58474600	-1.92741700
P	-0.28350600	-3.06125400	0.97355400
K	0.00050300	0.00004400	-0.00003200

Table SI-10 Total, ZP and Gibbs free energies of the structures optimized at wB97XD/6-31G(d,P)

File Name	SCF Energy (A.U)	SCF Energy (Kcal)	ZP Energy (A.U)	ZP Energy (Kcal)	Gibbs Free E (A.U)	Gibbs Free E (Kcal)
Li@AlN	-3574.248339	-2242874.788	-3574.168395	-2242824.622	-3574.216056	-2242854.53
Na@AlN	-3728.970568	-2339964.457	-3728.891231	-2339914.672	-3728.938216	-2339944.155
K@AlN	-4166.511685	-2614525.664	-4166.433717	-2614476.739	-4166.480176	-2614505.892
Li@AlP	-7013.401166	-4400975.859	-7013.353498	-4400945.947	-7013.415655	-4400984.951
Na@AlP	-7168.142768	-4498077.685	-7168.096743	-4498048.803	-7168.156963	-4498086.592
K@AlP	-7605.713743	-4772657.628	-7605.668116	-4772628.997	-7605.732037	-4772669.108
Li@BN	-963.2939362	-604476.0962	-963.162072	-604393.3502	-963.198225	-604416.0366
Na@BN	-1117.950316	-701524.4441	-1117.819328	-701442.2476	-1117.855245	-701464.7859
K@BN	-1555.327792	-975982.9653	-1555.200143	-975902.8641	-1555.235846	-975925.2681
Li@BP	-4401.885966	-2762225.262	-4401.811215	-2762178.355	-4401.858427	-2762207.981
Na@BP	-4556.615725	-2859319.655	-4556.538496	-2859271.193	-4556.586787	-2859301.496
K@BP	-4994.167097	-3133887.298	-4994.087965	-3133837.642	-4994.134822	-3133867.045
AlN	-3566.754278	-2238172.194	-3566.672665	-2238120.981	-3566.716802	-2238148.677
AlP	-7005.869996	-4396249.978	-7005.823492	-4396220.797	-7005.88226	-4396257.674
BN	-955.8823866	-599825.2784	-955.750189	-599742.3232	-955.784969	-599764.148
BP	-4394.357226	-2757500.906	-4394.280444	-2757452.724	-4394.325707	-2757481.127
Li	-7.489628262	-4699.812886	-7.489628	-4699.812721	-7.503031	-4708.223231
Na	-162.2522547	-101814.8312	-162.252255	-101814.8314	-162.267338	-101824.2961
K	-599.871698850	-376425.1898	-599.871699	-376425.1899	-599.887529	-376435.1234

Cartesian Coordinates of the geometries optimized at wB97XD/6-31G(d,p)

Li@AlN

Al	2.77463400	-0.22015900	0.37701100
Al	1.31461800	-1.34554500	2.08731200
Al	1.00488200	1.71442200	1.98511400
Al	1.04435300	-2.49664800	-0.75476900
Al	1.47014800	0.07142000	-2.39270500
Al	1.44899000	2.17793900	-1.02049900
Al	-1.47011000	-0.07127800	2.39415000
Al	-2.77696000	0.22120100	-0.37819400
Al	-1.31347900	1.34568100	-2.08713600
Al	-1.00437400	-1.71490000	-1.98668000
Al	-1.04331300	2.49717400	0.75429300
Al	-1.45024400	-2.17995600	1.02234700
N	-0.76769900	-2.81237900	-0.51088100
N	2.15203900	-1.95839600	0.54977900
N	0.80938900	-1.59626600	-2.35857600
N	2.13083700	0.31920800	2.03092200
N	2.63526700	0.75555900	-1.12187800
N	0.76835300	2.81491000	0.51163900
N	-0.80886800	1.59582100	2.35767700
N	-0.42292200	-1.60069600	2.45384300
N	-2.13000300	-0.31916500	-2.03056700
N	-2.15162100	1.95842100	-0.54985000
N	-2.63327600	-0.75455900	1.12072100
N	0.42341300	1.60097700	-2.45416600

Li	-0.00775300	-0.00520400	0.00206500

Na@AlN

Al	1.83996700	2.05138000	-0.67840600
Al	0.68386700	2.26402700	1.56750300
Al	-1.24507200	2.39807200	-0.86843700
Al	2.50448300	-0.24253900	1.31189600
Al	2.09417500	-0.87292600	-1.70505300
Al	0.22182800	0.44567300	-2.79321000
Al	-2.09437200	0.87280200	1.70493200
Al	-1.83939700	-2.05178700	0.67863900
Al	-0.68377000	-2.26425700	-1.56749600
Al	1.24491400	-2.39786300	0.86836600
Al	-2.50445600	0.24281700	-1.31228700
Al	-0.22211300	-0.44556500	2.79353100
N	1.31952000	-1.25068700	2.32971100
N	2.30813700	1.52636800	1.04271600
N	2.55814200	-1.47981500	-0.07532200
N	0.30183600	2.93782700	-0.12386000
N	1.87204200	0.93304000	-2.08851700
N	-1.31987100	1.25122200	-2.33020500
N	-2.55808000	1.47986600	0.07522400
N	-0.52313400	1.37502100	2.56392400
N	-0.30160800	-2.93868700	0.12364700
N	-2.30743800	-1.52588800	-1.04231600
N	-1.87213700	-0.93313200	2.08855400

N	0.52300600	-1.37496000	-2.56390800
Na	-0.00032900	0.00008500	0.00025100

K@AlN

Al	0.24062800	-2.35092300	1.63991000
Al	2.06071200	-2.00298000	-0.12875000
Al	-0.82678100	-2.41423300	-1.32909700
Al	1.97228400	0.24902000	2.07947900
Al	-1.13489800	0.30955700	2.62396800
Al	-2.52707100	-1.01241100	0.92954800
Al	1.13491400	-0.30936300	-2.62378200
Al	-0.24107400	2.35049900	-1.63999500
Al	-2.06089400	2.00294100	0.12859200
Al	0.82701600	2.41438100	1.32897600
Al	-1.97192500	-0.24893200	-2.07943200
Al	2.52711500	1.01258300	-0.92980000
N	2.38956000	1.54049300	0.79770000
N	1.90939300	-1.51350600	1.66720600
N	0.45899200	1.16931900	2.67078200
N	0.43377900	-2.91806000	-0.12967200
N	-1.25761300	-1.50534500	2.20747100
N	-2.38946200	-1.54047300	-0.79792500
N	-0.45879300	-1.16922500	-2.67085200
N	2.47168000	-0.79146800	-1.41138900
N	-0.43383000	2.91764500	0.12955100
N	-1.90986100	1.51362200	-1.66747300

N	1.25739400	1.50543000	-2.20759300
N	-2.47164200	0.79151900	1.41131900
K	0.00013100	-0.00007700	0.0005840

Li@AlP

Al	-1.05814800	-1.63750300	2.38338500
Al	-2.97786500	-0.46136600	0.78996500
Al	-0.90945100	1.73353000	2.37799900
Al	-1.07816200	-2.85611100	-0.74985700
Al	1.88623400	-2.34062500	0.81348700
Al	1.93566500	-0.08064700	2.39326600
Al	-2.15302000	0.13155900	-2.51970600
Al	-1.93068700	2.36301100	-0.76585100
Al	1.21289000	1.79955700	-2.50920400
Al	3.01834600	0.48982300	-0.74123200
Al	0.97308100	-1.94855600	-2.50108500
Al	1.08147200	2.80823900	0.79996800
P	1.12316000	-3.63393300	-0.92703600
P	2.35829100	-0.17838700	-2.87116800
P	3.65373800	-0.82160000	0.98321800
P	1.32812500	2.02888700	2.97889500
P	2.58984100	2.78258500	-0.93473700
P	-1.11828300	3.58084100	0.95299900
P	-2.43536800	0.15643800	2.96779500
P	-1.01086500	2.11033300	-2.89051300
P	-2.54839700	-2.75119500	0.96073400

P	-3.70043900	0.84496900	-0.95840800
P	-1.30932600	-1.95292700	-2.88269300
P	1.06850100	-2.16687900	2.98561200
Li	0.00357200	0.00039200	-0.83174300

Na@AlP

Al	-1.56627300	1.67522500	-2.22465400
Al	-1.09124300	-1.04144400	-2.82112600
Al	1.83420200	0.86001900	-2.46227400
Al	-3.15865300	-0.55257300	-0.00987800
Al	-1.71033600	2.41791900	1.20508800
Al	0.74183900	3.10169800	-0.00396400
Al	-0.73883700	-3.11988800	-0.00027000
Al	1.71506300	-2.41317900	-1.20724200
Al	1.57455200	-1.67295900	2.22743200
Al	1.09431500	1.04508700	2.81390400
Al	-1.84539000	-0.86127400	2.47517700
Al	3.14136600	0.55262900	0.01184900
P	-3.26839600	0.86964500	1.83390800
P	0.04184100	-0.81046400	3.75726700
P	0.24644400	3.09503300	2.27593100
P	2.67226500	2.55235400	-1.09217800
P	3.13214100	0.06322900	2.24232000
P	3.27080400	-0.86703800	-1.83473600
P	-0.04185900	0.81427200	-3.76478000
P	1.40329400	-3.48065900	0.84342800

P	-3.12543700	-0.06108700	-2.23739600
P	-0.24334300	-3.09102600	-2.27728400
P	-2.66359500	-2.54744000	1.08825100
P	-1.40060700	3.48517500	-0.84480200
Na	-0.02101000	-0.01965900	0.00895500

K@AlP

Al	-2.21408700	-2.47167800	0.17816400
Al	0.47666600	-3.23046200	-0.61718900
Al	-1.14707000	-0.94602300	-2.96867700
Al	0.30131100	-1.82643500	2.76139100
Al	-2.41492700	0.56584800	2.21162500
Al	-3.11752900	0.99296300	-0.57519200
Al	3.12271600	-0.99454600	0.57404700
Al	2.41369300	-0.56558700	-2.21272800
Al	2.21344900	2.47392200	-0.18120900
Al	-0.47816300	3.22945000	0.61388500
Al	1.14716400	0.94750500	2.97346300
Al	-0.30208800	1.82449600	-2.75642100
P	-0.82107400	-0.03702700	3.75642900
P	1.41995900	2.99040800	1.95289500
P	-2.64013500	2.58635700	1.06296000
P	-2.47441900	0.96620500	-2.78260600
P	0.55863900	3.51621400	-1.45852000
P	0.81961500	0.03751700	-3.75621400
P	-1.42230100	-2.99225200	-1.95581600

P	3.67245100	0.80836900	-0.80501200
P	-0.55936100	-3.51270600	1.45603500
P	2.63906000	-2.58613100	-1.06440600
P	2.47256100	-0.96536600	2.78028600
P	-3.67379100	-0.80790900	0.80357800
K	0.00616800	-0.00253200	0.00741200

Li@BN

B	-0.87376600	-0.44346400	-1.98905900
B	-0.86563000	1.80258700	-0.96029300
B	0.87940800	0.41971700	-1.98192700
B	0.89189600	-1.78790400	-0.96394200
B	1.37498900	1.74349200	-0.00026100
B	2.21891000	0.00241400	-0.00026400
B	0.87987900	0.41994100	1.98166500
B	0.89210100	-1.78780000	0.96394900
B	-0.86540600	1.80269700	0.96028500
B	-0.87328100	-0.44322900	1.98933400
B	-1.36943100	-1.73680800	0.00024200
B	-2.55719400	0.01098100	0.00032200
N	-1.87049900	-0.93475200	-1.11837000
N	-1.88984700	1.41246100	0.00013900
N	-1.87019000	-0.93458900	1.11888300
N	0.11445800	2.42305500	-0.00015300
N	-0.47355300	1.00372900	2.10961900
N	1.92347900	0.92822100	1.12124500

N	1.92321400	0.92809300	-1.12180800
N	-0.47406000	1.00348000	-2.10962200
N	-0.05606600	-2.39701300	0.00014300
N	1.96604900	-1.41550800	-0.00014000
N	0.51527700	-1.01139000	-2.11717600
N	0.51577900	-1.01115300	2.11719400
Li	-0.31022200	0.00814100	0.00002400

Na@BN

B	0.88305100	-0.47182600	2.00525900
B	0.92527500	1.79855100	0.96822900
B	-0.87325300	0.44862900	2.01615100
B	-0.94166100	-1.79343300	0.98076100
B	-1.35127000	1.80581400	0.00065100
B	-2.25134600	0.05563600	0.00251400
B	-0.87793800	0.44659200	-2.01460200
B	-0.94392700	-1.79437000	-0.97687900
B	0.92313600	1.79760700	-0.97201100
B	0.87812200	-0.47352600	-2.00688400
B	1.34349600	-1.77835200	-0.00083100
B	2.55342700	-0.04536100	-0.00284400
N	1.86083800	-0.98783600	1.12436800
N	1.93613900	1.38905500	-0.00283000
N	1.85809200	-0.98876600	-1.12783000
N	-0.05824800	2.42772000	-0.00111300
N	0.49929300	0.99149000	-2.12048400
N	-1.90396700	0.97438700	-1.12225900

N	-1.90134700	0.97547300	1.12563200
N	0.50425000	0.99346900	2.11839600
N	-0.00267500	-2.40736400	0.00112900
N	-2.00067500	-1.37035200	0.00293800
N	-0.53585600	-1.00092200	2.12241900
N	-0.54087300	-1.00298800	-2.12034100
Na	0.05996900	0.00605800	0.00020500

K@BN

B	-2.56918400	0.05638700	0.00003900
B	-0.91919000	-0.45585600	-2.05151000
B	-1.44340300	-1.77532900	0.00004100
B	-0.91914800	-0.45579000	2.05154300
B	0.89037700	-1.86517300	-1.00030700
B	0.89039100	-1.86516500	1.00028300
B	2.29369800	-0.03015000	0.00000200
B	0.90708300	0.42380600	2.05940400
B	0.90706600	0.42381100	-2.05940700
B	1.44784600	1.78852000	0.00000700
B	-0.86987900	1.87976700	0.99207400
B	-0.86992200	1.87973600	-0.99212400
N	-1.90180800	1.51159200	-0.00001100
N	-0.47199200	1.01982300	-2.14979200
N	0.15493800	2.45302400	-0.00003200
N	0.50275200	-1.03072100	-2.14894000
N	1.95907200	0.91229400	-1.13412400
N	1.96209500	-1.46159200	-0.00001800

N	-0.08400800	-2.43734200	0.00000400
N	-1.91717100	-0.94321800	-1.14229300
N	-0.47194000	1.01989400	2.14976000
N	0.50276100	-1.03073000	2.14891900
N	-1.91714200	-0.94314800	1.14238500
N	1.95907500	0.91226400	1.13416200
K	-0.03500600	0.00537900	-0.00001900

Li@BP

B	0.62993800	0.73260200	-2.53635200
B	0.99049400	-2.03974300	-1.48537100
B	-1.41783000	-0.45467400	-2.27104100
B	-1.37358200	2.17577000	-0.85400800
B	-1.51904400	-2.24383300	0.11941000
B	-2.67320500	-0.18705400	0.42740600
B	-0.62618800	-0.72956100	2.52937600
B	-0.98923600	2.03820600	1.48612300
B	1.37293500	-2.17331700	0.85522600
B	1.41212400	0.45243000	2.26170100
B	1.51700900	2.23947000	-0.11882500
B	2.66801100	0.18702700	-0.42644000
P	-2.67293100	-1.32948800	-1.12868900
P	-2.20109600	-1.49781900	1.76344700
P	0.11270300	-3.18335500	-0.20259800
P	0.25344800	-1.10691500	-2.98113300
P	-1.16872200	1.43009500	-2.60123100

P	2.63836200	-1.72148500	-0.53173700
P	2.20011500	1.49752700	-1.76487200
P	2.67742600	1.33151900	1.12930300
P	-0.11341200	3.18518100	0.20307300
P	-2.63756500	1.71990600	0.53163000
P	-0.25399100	1.10910700	2.98520400
P	1.17078800	-1.43284400	2.60494400
Li	-0.01132400	-0.00267900	-0.01537800

Na@BP

 # opt freq uwb97xd/6-31g(d,p) nosymm geom=connectivity

scf=(xqc,fermi,novaracc)

B	2.68606000	-0.42166900	0.26157000
B	1.35365500	-0.08625900	-2.39380400
B	2.03821300	1.80643900	-0.18335700
B	1.09382200	0.86068600	2.72534700
B	-0.59081000	2.10276700	-1.65637900
B	-0.78797400	2.50061000	0.73386500
B	-2.70112400	0.42560500	-0.31877600
B	-1.33656800	0.08598800	2.37904600
B	-0.96946700	-0.77213800	-2.46093600
B	-2.04394000	-1.83792800	0.13241200
B	0.54601500	-2.09616500	1.65067800
B	0.75402600	-2.53036700	-0.73210300
P	0.60895400	3.04695600	-0.49546700

P	-2.18392600	2.23733800	-0.58279300
P	-0.18124900	0.87768400	-3.06181500
P	2.85187900	0.54578400	-1.41082100
P	2.56043900	1.03582400	1.46954900
P	0.61354200	-1.86625100	-2.51634500
P	2.14165900	-2.23682300	0.55857700
P	-0.64205500	-3.07714800	0.47664200
P	0.18729700	-0.87447700	3.02869000
P	-0.60451600	1.85239100	2.48499700
P	-2.82462300	-0.55415900	1.33030100
P	-2.61557700	-1.06539800	-1.54218600
Na	0.04768600	0.04209400	0.12287700

K@BP

 # opt freq uwb97xd/6-31g(d,p) nosymm geom=connectivity

scf=(xqc,fermi,novaracc)

B	-1.30843500	2.57447800	-0.00014700
B	-0.00206100	1.25501400	2.45847400
B	1.29980000	2.57861600	-0.00011500
B	-0.00200600	1.25476700	-2.45859400
B	2.51533800	-0.01571200	1.20268300
B	2.51538200	-0.01582700	-1.20263300
B	1.24016400	-2.49275000	0.00013100
B	0.00190000	-1.21784800	-2.47654400

B	0.00183200	-1.21757900	2.47668800
B	-1.23207800	-2.49710600	0.00012100
B	-2.51516700	-0.02402100	-1.20267000
B	-2.51520000	-0.02388900	1.20259900
P	2.85760600	1.44211500	-0.00003400
P	2.87439700	-1.50125800	0.00010300
P	1.45816900	0.00922700	2.80913900
P	-0.00463900	2.81797300	1.41127400
P	-0.00460500	2.81784700	-1.41156300
P	-1.45834300	0.00460000	2.80918800
P	-2.86248400	1.43276500	-0.00011900
P	-2.86925100	-1.51058400	0.00004100
P	-1.45825800	0.00430000	-2.80921000
P	1.45823600	0.00893300	-2.80910300
P	0.00462100	-2.83848000	-1.45300800
P	0.00460500	-2.83833000	1.45328800
K	0.00009700	0.07750900	0.00000500

AlN

Al	2.12115200	1.28356900	-1.20496200
Al	0.42173300	2.72036600	-0.12871800
Al	-0.62238400	1.09960100	-2.44893800
Al	1.89791800	0.90912800	1.78020600
Al	2.32542500	-1.48069300	-0.01208500
Al	1.06091900	-1.38398100	-2.13324300
Al	-1.06091100	1.38399900	2.13323300
Al	-2.32540000	1.48076100	0.01206600

Al	-2.12119000	-1.28362300	1.20495600
Al	-0.42175700	-2.72043300	0.12875600
Al	0.62235600	-1.09959100	2.44883600
Al	-1.89786500	-0.90910100	-1.78010700
N	0.41484300	0.69000100	2.85958700
N	2.05928400	2.09330100	0.45410400
N	2.28651700	-0.89404900	1.67350500
N	0.66616100	2.19817600	-1.88389600
N	2.51871600	-0.42805900	-1.51897200
N	-0.41484700	-0.69000400	-2.85958800
N	-2.28650300	0.89406700	-1.67350700
N	-1.11205300	2.64208300	0.78179300
N	-0.66618700	-2.19820600	1.88392800
N	-2.05930200	-2.09335900	-0.45410800
N	-2.51864800	0.42804500	1.51890200
N	1.11202600	-2.64200000	-0.78175000

AlP

Al	0.00000000	1.40536100	-2.85837000
Al	0.00000000	-1.40536100	-2.85837000
Al	2.85912200	0.00000000	-1.40523800
Al	-2.85912200	0.00000000	-1.40523800
Al	-1.40527200	2.85871100	-0.00041800
Al	1.40527200	2.85871100	-0.00041800
Al	-1.40527200	-2.85871100	-0.00041800
Al	1.40527200	-2.85871100	-0.00041800
Al	0.00000000	-1.40522100	2.85885200

Al	0.00000000	1.40522100	2.85885200
Al	-2.85822900	0.00000000	1.40530900
Al	2.85822900	0.00000000	1.40530900
P	-3.40129500	1.76828100	0.00016100
P	-1.76832700	0.00000000	3.40160800
P	0.00000000	3.40095700	1.76793700
P	3.40129500	1.76828100	0.00016100
P	1.76832700	0.00000000	3.40160800
P	3.40129500	-1.76828100	0.00016100
P	1.76819000	0.00000000	-3.40098100
P	0.00000000	-3.40095700	1.76793700
P	-1.76819000	0.00000000	-3.40098100
P	0.00000000	-3.40179300	-1.76864000
P	-3.40129500	-1.76828100	0.00016100
P	0.00000000	3.40179300	-1.76864000

BN

B	-0.19286200	-0.67572700	2.06171900
B	1.16014800	-1.79444200	0.42548600
B	1.41046900	0.26102700	1.63958400
B	-0.56915200	1.59293800	1.37352400
B	2.07057300	0.14093000	-0.66422700
B	1.23009600	1.78712300	-0.20470200
B	0.19285800	0.67573400	-2.06171400
B	-1.16014400	1.79443100	-0.42548800
B	0.56915900	-1.59294600	-1.37352800
B	-1.41047500	-0.26101800	-1.63958300

B	-2.07057400	-0.14093300	0.66422800
B	-1.23009300	-1.78712700	0.20470000
N	-1.43728500	-1.16190900	1.53059100
N	-0.00926900	-2.38540200	-0.26424500
N	-2.13495400	-0.92480600	-0.58987400
N	1.88132600	-1.28107700	-0.76169000
N	-0.16367700	-0.74541000	-2.27505000
N	1.43728700	1.16190500	-1.53059300
N	2.13495500	0.92480200	0.58987200
N	1.15406700	-1.19449600	1.73204300
N	-1.88131800	1.28107200	0.76169000
N	0.00927200	2.38539000	0.26424100
N	0.16367600	0.74542300	2.27507600
N	-1.15408200	1.19451400	-1.73206100

BP

B	1.18096100	2.41921400	-0.00033500
B	0.00000000	1.18118800	-2.41890400
B	-1.18096100	2.41921400	-0.00033500
B	0.00000000	1.18080300	2.41927700
B	-2.41917400	0.00000000	-1.18095200
B	-2.41905300	0.00000000	1.18104800
B	-1.18096100	-2.41921400	-0.00033500
B	0.00000000	-1.18080300	2.41927700
B	0.00000000	-1.18118800	-2.41890400
B	1.18096100	-2.41921400	-0.00033500

B	2.41905300	0.00000000	1.18104800
B	2.41917400	0.00000000	-1.18095200
P	-2.82554500	1.46037800	0.00010300
P	-2.82554500	-1.46037800	0.00010300
P	-1.46025100	0.00000000	-2.82538100
P	0.00000000	2.82617800	-1.46068800
P	0.00000000	2.82506900	1.46010700
P	1.46025100	0.00000000	-2.82538100
P	2.82554500	1.46037800	0.00010300
P	2.82554500	-1.46037800	0.00010300
P	1.46046500	0.00000000	2.82582200
P	-1.46046500	0.00000000	2.82582200
P	0.00000000	-2.82506900	1.46010700
P	0.00000000	-2.82617800	-1.46068800