NXAl$_3^+$ (X=N, P, As): Penta-atomic planar tetracoordinate nitrogen with N–X multiple bonding

Supporting Information.

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SI1: Full citations for reference.

SI2: The structures of the isomer and transition of NXAl$_3^+$ (X=N, P, As).

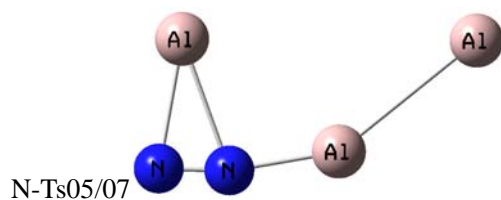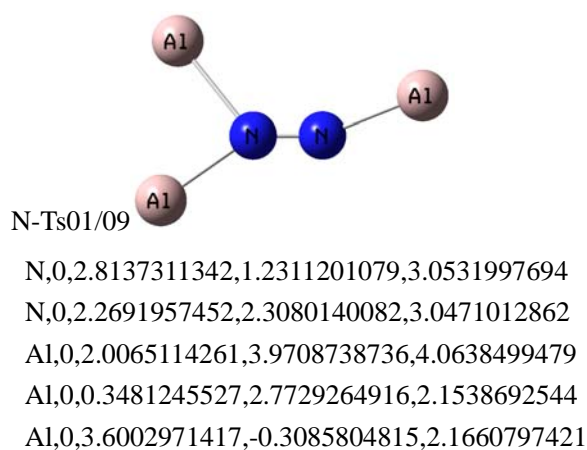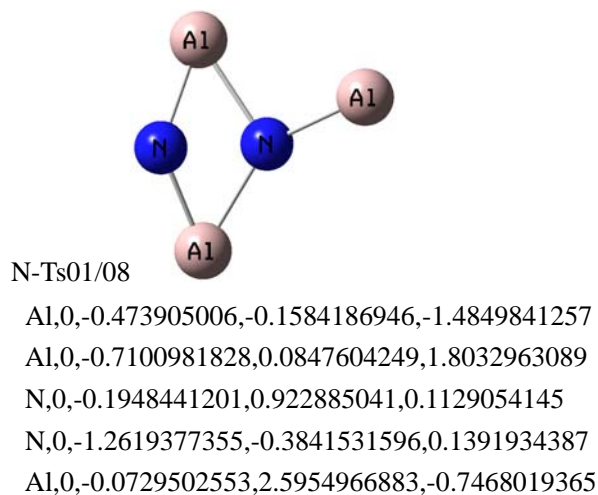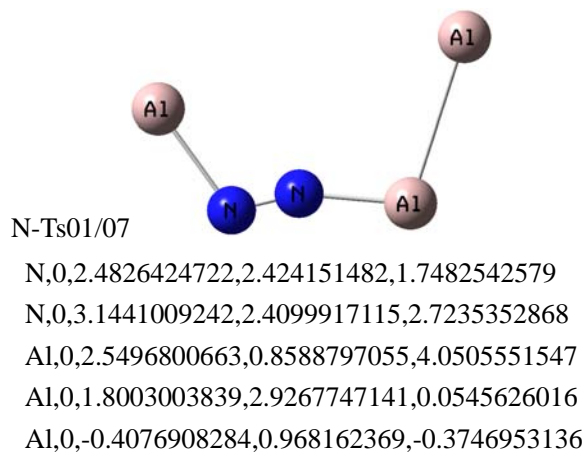**SI3: The details of MD simulations.**

SI1 Full citations for reference 19.

Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Montgomery JA Jr, Vreven T, Kudin KN, Burant JC, Millam JM, Iyengar SS, Tomasi J, Barone V, Mennucci B, Cossi M, Scalmani G, Rega N, Petersson GA, Nakatsuji H, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Klene M, Li X, Knox JE, Hratchian HP, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Ayala PY, Morokuma K, Voth GA, Salvador P, Dannenberg JJ, Zakrzewski VG, Dapprich S, Daniels AD, Strain MC, Farkas O, Malick DK, Rabuck AD, Raghava-chari K, Foresman JB, Ortiz JV, Cui Q, Baboul AG, Clifford S, Cioslowski J, Stefanov BB, Liu G, Liashenko A, Piskorz P, Komaromi I, Martin RL, Fox DJ, Keith T, Al-Laham MA, Peng CY, Nanayakkara A, Challacombe M, Gill PMW, Johnson B, Chen W, Wong MW, Gonzalez C, Pople JA, *Gaussian 03, Revision D.02.* Gaussian Inc., Wallingford CT, 2004.

Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenberg JL, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery JA, Peralta JE Jr, Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Rega N, Millam JM, Klene M, Knox JE, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Martin RL, Morokuma K, Zakrzewski

VG, Voth GA, Salvador P, Dannenberg JJ, Dapprich S, Daniels AD, Farkas O, Foresman JB, Ortiz JV, Cioslowski J, and Fox DJ, *Gaussian 09, Revision A.01.* Gaussian, Inc., Wallingford CT, 2009.

SI2-1 Optimized geometries of interconversion transition states of $N_2Al_3^+$, $NPAl_3^+$

and $NAsAl_3^+$ at the B3LYP/aug-cc-pVTZ level, respectively.

N-Ts01/07

N,0,2.4826424722,2.424151482,1.7482542579
N,0,3.1441009242,2.4099917115,2.7235352868
Al,0,2.5496800663,0.8588797055,4.0505551547
Al,0,1.8003003839,2.9267747141,0.0545626016
Al,0,-0.4076908284,0.968162369,-0.3746953136

N-Ts01/08

Al,0,-0.473905006,-0.1584186946,-1.4849841257
Al,0,-0.7100981828,0.0847604249,1.8032963089
N,0,-0.1948441201,0.922885041,0.1129054145
N,0,-1.2619377355,-0.3841531596,0.1391934387
Al,0,-0.0729502553,2.5954966883,-0.7468019365

N-Ts01/09

N,0,2.8137311342,1.2311201079,3.0531997694
N,0,2.2691957452,2.3080140082,3.0471012862
Al,0,2.0065114261,3.9708738736,4.0638499479
Al,0,0.3481245527,2.7729264916,2.1538692544
Al,0,3.6002971417,-0.3085804815,2.1660797421

N-Ts05/07

Al,0,-0.3005978429,-0.590543056,-1.6630827809
Al,0,-0.6550458006,1.3121836721,0.9079703572
N,0,-1.4004955355,-0.296254385,0.3696995775
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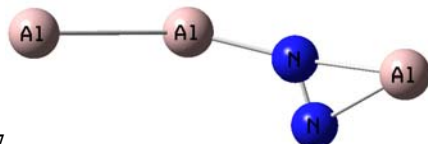
N-Ts06/07

N,0,1.6871953561,0.8659542287,1.5409058408
N,0,2.3227315129,-0.1739053561,1.4818746288
Al,0,4.4483326965,4.7427241,0.7408484359
Al,0,2.5926654805,2.5199116808,2.0657203301
Al,0,0.6074769539,-0.5855796534,0.3201977645
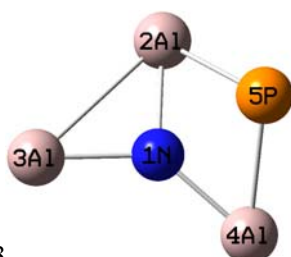
P-Ts01/03

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Al,0,-0.603977094,0.3460874903,-2.4180456932
Al,0,0.2153364086,-1.808203866,0.2850054989
N,0,-0.1201724192,-0.1753082611,-0.6343971787
P,0,-0.7546973735,0.031879121,1.301075791
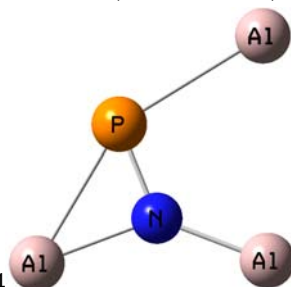
P-Ts01/04

Al,0,2.5053342056,-0.8709166801,0.
Al,0,-2.5077299471,0.4526340028,0.
Al,0,0.7380384649,2.296546647,0.
N,0,-0.4623897542,0.8020982881,0.
P,0,-0.2257838993,-0.8105928477,0.
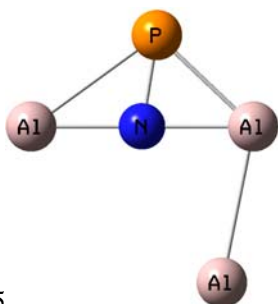
P-Ts01/05

Al,0,-1.7759440297,-1.5580949503,0.
Al,0,-0.7007233797,2.6928666325,0.
P,0,0.9993490297,-1.5425858003,0.
N,0,-0.1861471246,-0.3879934194,0.
Al,0,1.4058179943,0.7900460475,0.
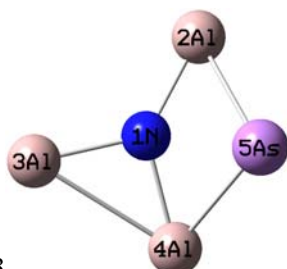
As-Ts01/03

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Al,0,-1.7530305296,-0.270659833,-2.0317169647
Al,0,0.0245743464,-1.6897694856,-0.3550227667
N,0,-0.5434620662,0.1757434283,-0.5794974156
As,0,-0.2921025519,-0.0719611167,1.507418896
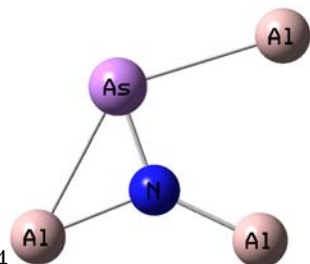
As-Ts01/04

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Al,0,-2.4800893558,0.6241376231,0.
Al,0,0.7570937594,2.2035817925,0.
N,0,-0.4474740059,0.7344008194,0.
As,0,-0.2764306892,-1.0393955989,0.
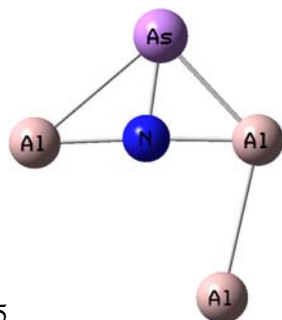
As-Ts01/05

N,0,-0.3357606078,-0.4925751295,0.
Al,0,0.9812504646,0.9321518082,0.
As,0,1.1356035244,-1.5517826183,0.
Al,0,-1.7308615383,-1.841557424,0.
Al,0,-1.4456598429,2.3863093635,0.

The figure means a fixed bond angle scanning between **N-03** and **N-05**, **N-04** and

N-05 isomers at the B3LYP/6-311+G(d) level.
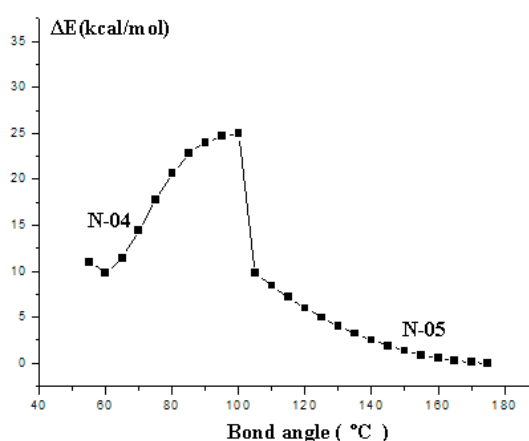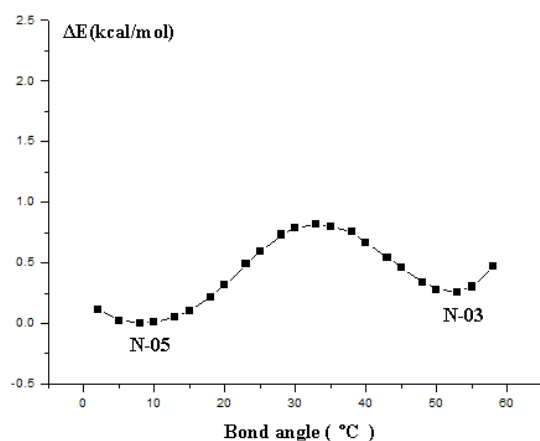
SI2-2 Calculated structures for the isomer of the $N_2Al_3^+$, $NPAl_3^+$ and $NAsAl_3^+$ in both the singlet and triplet electronic states at the B3LYP/6-311+G(d) level, respectively.

SI2-2-1: $N_2Al_3^+$
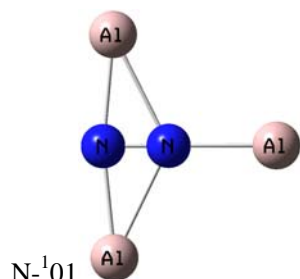
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Al,0,0.,0.,2.3572303843
Al,0,0.,2.1273061328,-0.7476192599
N,0,0.,0.,0.3229678281
N,0,0.,0.,-0.9115289327

N-^{1}03
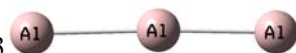
N,0,2.3352726365,-0.4471776948,0.
Al,0,-4.2854544343,-1.0197118553,0.
Al,0,-1.6320528523,0.5866161246,0.
N,0,3.0871135597,-1.2445173521,0.
Al,0,0.9482023504,2.2732287277,0.
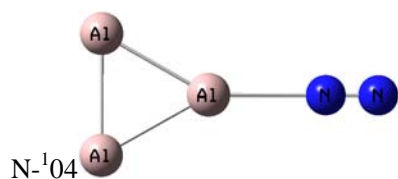
N-^{1}04

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Al,0,0.,0.,0.2400273717
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N,0,0.,0.,-3.2985567445
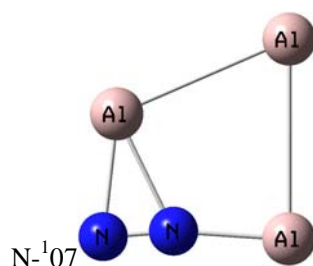Al,0,0.,-1.2683769906,2.4720892331
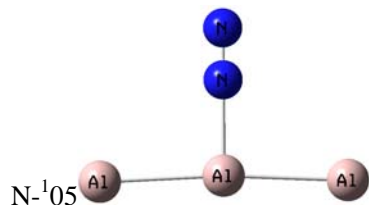
N-^{1}05

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Al,0,2.9798109875,-1.8271456036,0.
N,0,-2.0316496734,-1.7438083913,0.
Al,0,1.0622772959,0.5750654763,0.
N,0,-1.1535601722,-1.086277108,0.

N-[1]06
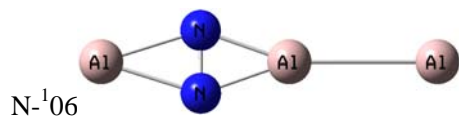
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Al,0,-0.6685484979,3.8286999001,0.
N,0,0.7080933871,-0.8804034635,0.
N,0,-0.5478795509,-1.0759862025,0.
Al,0,-0.2004128622,0.8232412331,0.

N-[1]07

Al,0,-0.3241236059,-1.5394405348,0.
Al,0,0.3992655614,1.974711258,0.
N,0,-0.9499393051,0.5670225767,0.
N,0,-1.8887962835,-0.1647042009,0.
Al,0,2.6781102831,-0.5166619189,0.

N-[1]08
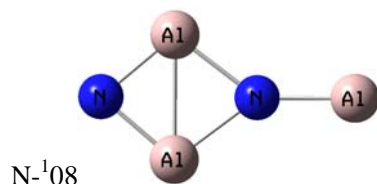
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N,0,0.,0.,-0.6241668983
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Al,0,-1.155319259,0.,0.8867669841

N-[1]09
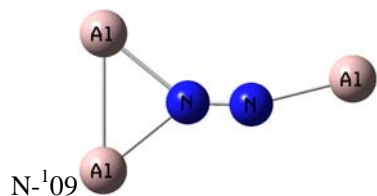
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N,0,-0.6062892322,-0.6576888568,0.
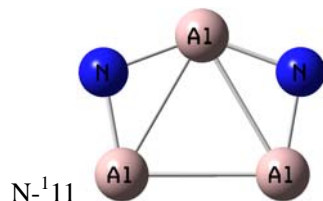
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N-^{1}10
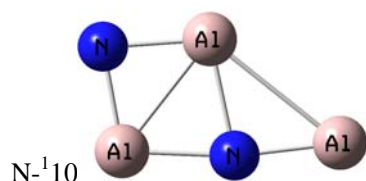
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N,0,0.,0.1957402362,-2.0486032272
Al,0,0.,-1.2349766722,-1.0144780395

N-^{1}11

Al,0,0.,0.,1.326431602
Al,0,0.,1.3416820054,-0.9818105579
Al,0,0.,-1.3416820054,-0.9818105579
N,0,0.,1.6421877494,0.7198575868
N,0,0.,-1.6421877494,0.7198575868

N-^{1}12

N,0,0.,0.,-4.9206561774
Al,0,0.,0.,-3.165345359
Al,0,0.,0.,-0.5861117375
Al,0,0.,0.,1.9930648905
N,0,0.,0.,3.7483340334

N-^{1}13

N,0,4.4348067781,0.0811390247,0.
Al,0,2.6698465219,0.0714912172,0.
Al,0,0.0961327291,0.0619292524,0.
N,0,-1.5797281996,-0.1251070754,0.
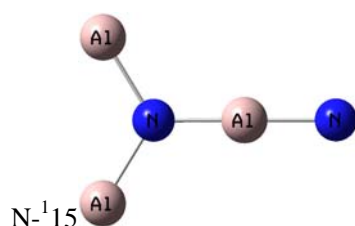Al,0,-3.2817058195,0.2342124912,0.

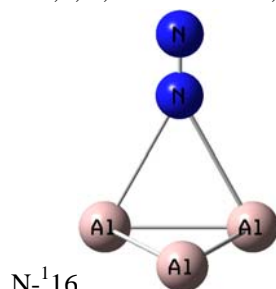N-^{1}14
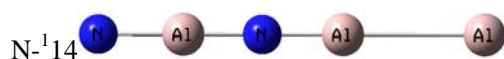
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N,0,0.,0.,-0.138927915
N,0,0.,0.,-3.6575590664
Al,0,0.,0.,-1.8332226604

N-^{1}15

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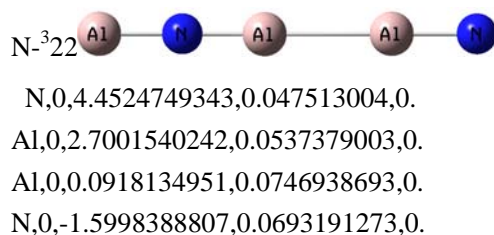N,0,0.,0.,2.7098750043
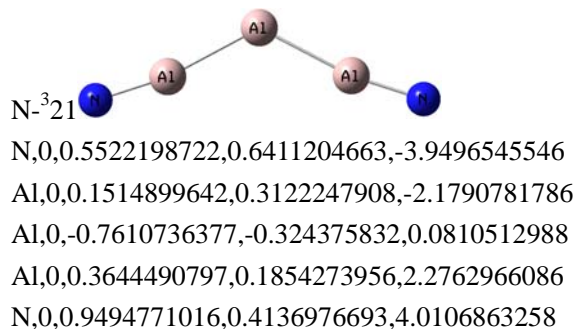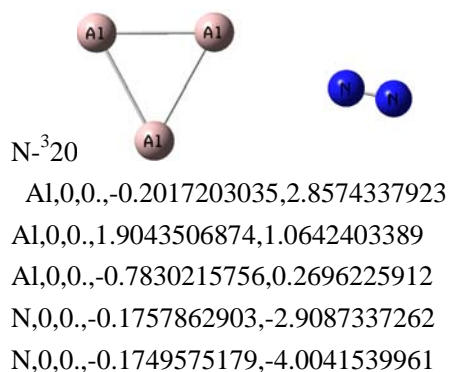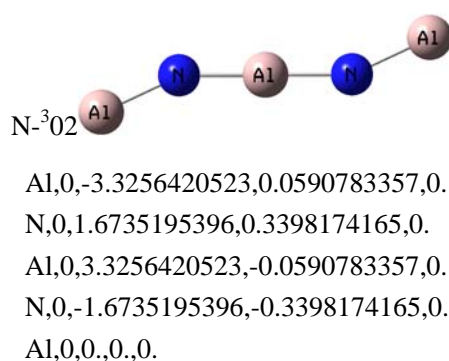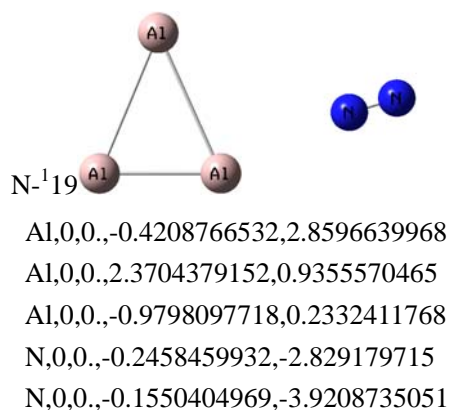Al,0,0.,1.6182724476,-1.8403541355

N-^{1}16

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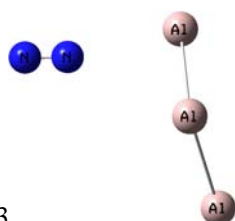Al,0,0.2628451223,-1.1622716491,1.2787790516

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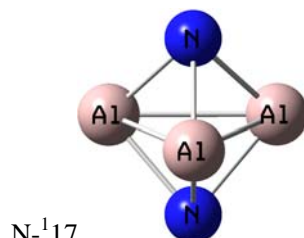
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Al,0,1.215629676,-0.7018441179,0.
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Al,0,-1.2156296736,-0.7018441221,0.
N,0,0.,0.,1.31899443

N-^{1}18
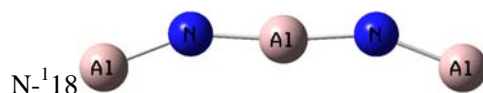
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Al,0,0.,-3.3077305816,-0.2324963241
N,0,0.,1.711601405,0.3904986406
Al,0,0.,0.,0.2937933668

N-^{1}19

Al,0,0.,-0.4208766532,2.8596639968
Al,0,0.,2.3704379152,0.9355570465
Al,0,0.,-0.9798097718,0.2332411768
N,0,0.,-0.2458459932,-2.829179715
N,0,0.,-0.1550404969,-3.9208735051

N-^{3}02

Al,0,-3.3256420523,0.0590783357,0.
N,0,1.6735195396,0.3398174165,0.
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N,0,-1.6735195396,-0.3398174165,0.
Al,0,0.,0.,0.

N-^{3}20

Al,0,0.,-0.2017203035,2.8574337923
Al,0,0.,1.9043506874,1.0642403389
Al,0,0.,-0.7830215756,0.2696225912
N,0,0.,-0.1757862903,-2.9087337262
N,0,0.,-0.1749575179,-4.0041539961

N-^{3}21

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Al,0,0.1514899642,0.3122247908,-2.1790781786
Al,0,-0.7610736377,-0.324375832,0.0810512988
Al,0,0.3644490797,0.1854273956,2.2762966086
N,0,0.9494771016,0.4136976693,4.0106863258

N-^{3}22

N,0,4.4524749343,0.047513004,0.
Al,0,2.7001540242,0.0537379003,0.
Al,0,0.0918134951,0.0746938693,0.
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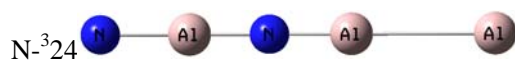Al,0,-3.3052515628,0.078401009,0.

N-³23

N,0,0.1676077139,-2.6308552599,0.0307594325
Al,0,-1.9976963979,2.6574732189,0.4527302771
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N,0,-0.3036905752,-3.6168602886,-0.0497407493
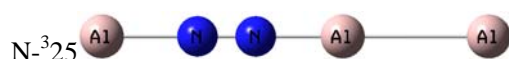Al,0,2.0662797171,-0.3780779716,0.4825268634

N-³24

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Al,0,0.,0.,1.595955876
N,0,0.,0.,-0.1264558123
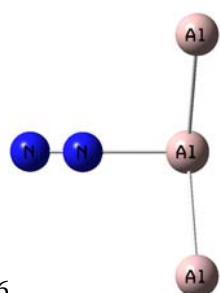N,0,0.,0.,-3.680006157
Al,0,0.,0.,-1.8060721269

N-³25

Al,0,0.0540240665,3.8358096536,0.
Al,0,-0.0343696053,-4.0984292654,0.
N,0,0.,0.675435167,0.
N,0,0.0145705438,1.8693950131,0.
Al,0,-0.0275001387,-1.1076735621,0.

N-³26

Al,0,2.6052278206,-0.9558073385,-0.31371328
Al,0,-2.6062476365,-0.9565666765,-0.3138267704
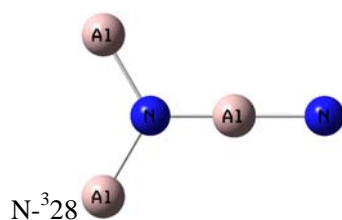N,0,0.0020368065,2.7364039719,-0.0973790828
Al,0,-0.0009266692,-0.482958194,0.6597164808
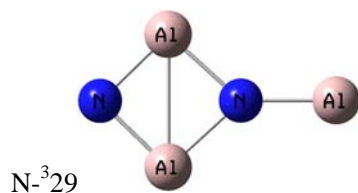N,0,0.0003256787,1.6417822371,0.0560736523
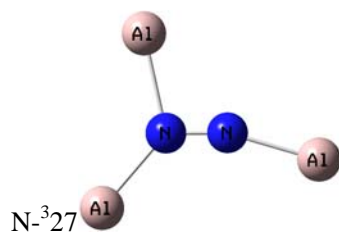
N-³27

Al,0,-1.7906239272,-1.9443263197,0.
Al,0,-0.4050367187,2.3662813563,0.
N,0,0.3495424031,0.4411771563,0.
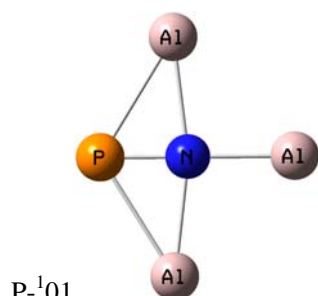N,0,-0.5568731277,-0.4305718023,0.
Al,0,2.3175080205,-0.1116332106,0.

N-^{3}28

Al,0,0.,0.,0.8760890757
Al,0,0.,-1.6762761116,-1.8334635666
N,0,0.,0.,-0.8601566321
N,0,0.,0.,2.7492327396
Al,0,0.,1.6762761116,-1.8334635666

N-^{3}29

Al,0,1.2646520961,0.,0.8529357045
Al,0,0.,0.,-2.3509695331
N,0,0.,0.,-0.5280130277
N,0,0.,0.,2.141188092
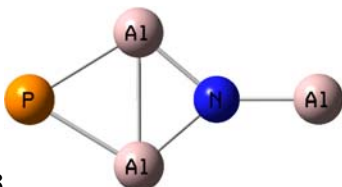Al,0,-1.2646520961,0.,0.8529357045

SI2-2-2: NPAl$_3^+$

P-^{1}01

Al,0,0.,-2.2411906545,-0.1770385418
Al,0,0.,0.,2.0702507879
Al,0,0.,2.2411906545,-0.1770385418
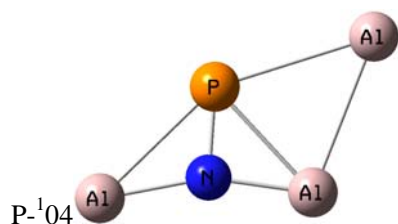N,0,0.,0.,0.0878611531
P,0,0.,0.,-1.5306040973

P-^{1}03

Al,0,-0.0306709303,0.3749968304,-1.1980997027
Al,0,-0.0053820298,-2.8763879695,0.
N,0,-0.0558071021,-1.0334393313,0.
P,0,0.0020200124,2.3280698599,0.
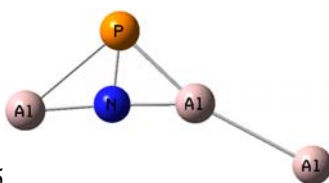Al,0,-0.0306709303,0.3749968304,1.1980997027

P-^{1}04

N,0,0.9480162721,0.3239892056,0.
Al,0,-2.9163634497,-0.3997836705,0.
Al,0,-0.5737052408,1.4990342779,0.
Al,0,2.922442216,-0.0318986679,0.
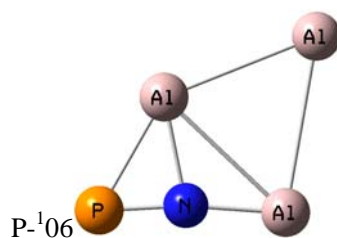P,0,0.0403608124,-1.0431980352,0.

P-^{1}05

Al,0,-0.6603378782,-2.884385537,0.
Al,0,-1.2311030442,3.5848613681,0.

P,0,1.6031919852,-0.8830908135,0.
N,0,-0.063545788,-1.0104603287,0.
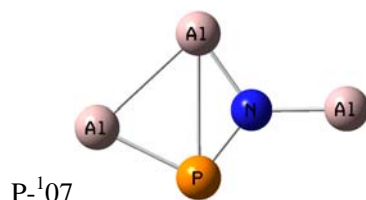Al,0,0.0388507252,0.8832143111,0.

P-[1]06

Al,0,-0.1251573464,-1.2896246157,0.
Al,0,0.4680636284,1.8185202649,0.
N,0,-0.9362637167,0.5932570972,0.
P,0,-2.3016153176,-0.2567913891,0.
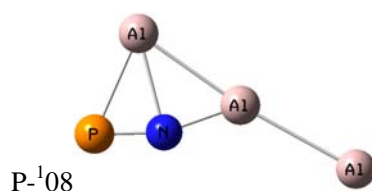Al,0,2.8094894023,-0.5444341773,0.

P-[1]07

Al,0,1.6363284712,-0.157548621,0.
N,0,-0.0002558864,0.7451928281,0.
Al,0,-0.0314072309,-2.3644096686,0.
P,0,-1.2436088026,-0.4500023708,0.
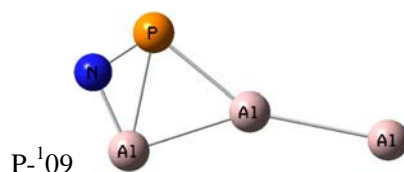Al,0,-0.1703968714,2.6430297824,0.

P-[1]08

N,0,-0.0010293812,0.8917135741,0.
Al,0,2.8191773414,-2.5064291632,0.
Al,0,0.2822835128,-0.9170145531,0.
Al,0,-2.2598025154,0.3106767469,0.
P,0,-0.7232369576,2.2917753953,0.
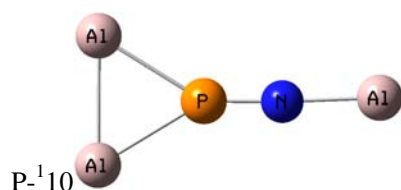
P-[1]09

Al,0,-0.0246722966,3.9236193469,0.
Al,0,1.4285670664,-1.5347672553,0.
N,0,-0.0728185645,-2.6647943534,0.
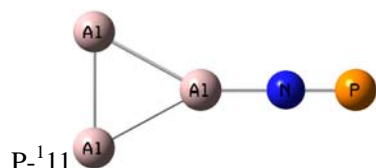Al,0,0.0264713088,0.8500901945,0.
P,0,-1.2071529141,-1.5674404627,0.

P-^{1}10

Al,0,0.,1.278666,2.078348
N,0,0.,-0.037572,-1.502366
Al,0,0.,-1.264908,2.103748
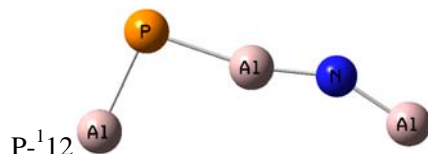Al,0,0.,0.02593,-3.409862
P,0,0.,-0.017463,0.031834

P-^{1}11

Al,0,0.,1.2578234072,2.3521129662
Al,0,0.,0.,0.0548440761
N,0,0.,0.,-1.7842297061
P,0,0.,0.,-3.2914719326
Al,0,0.,-1.2578234072,2.3521129662

P-^{1}12

Al,0,-0.2626900126,-0.3965675595,0.
N,0,-1.9717023861,-0.3864351628,0.
Al,0,-3.4997181323,0.427474735,0.
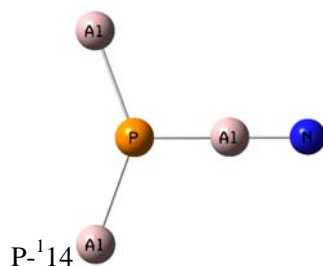P,0,1.893968183,-0.9131686035,0.
Al,0,2.6312595981,1.1888043008,0.

P-^{1}13

Al,0,0.,0.,4.6903806932
Al,0,0.,0.,1.6867759267
N,0,0.,0.,-0.0352798024
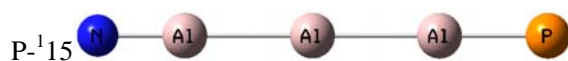P,0,0.,0.,-4.0078389801
Al,0,0.,0.,-1.7309122374

P-^{1}14

Al,0,0.,2.4603717577,1.4383139148

Al,0,0.,-2.4603717577,1.4383139148
N,0,0.,0.,-3.4451063414
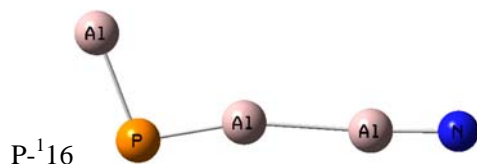Al,0,0..0.,-1.6502202444
P,0,0..0.,0.5419771463

P-^{1}15

N,0,0.,0.,-4.9845640091
Al,0,0.,0.,-3.2326112783
Al,0,0.,0.,-0.6682247639
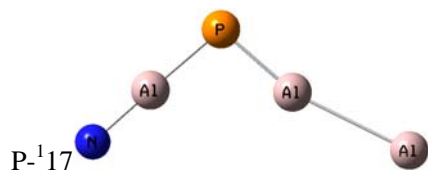Al,0,0.,0.,1.8862622249
P,0,0.,0.,4.0684234764

P-^{1}16

N,0,4.4387482003,0.3802366864,0.
Al,0,2.6963443704,0.0775226917,0.
Al,0,0.1588595542,-0.2112167814,0.
P,0,-1.875120606,-0.9488348488,0.
Al,0,-3.0794795089,1.0259571621,0.

P-^{1}17

N,0,3.3651078739,-1.6888498169,0.
Al,0,2.2342211526,-0.2716126715,0.
Al,0,-3.9589066533,-0.6665632237,0.
P,0,0.8394521302,1.4070459152,0.
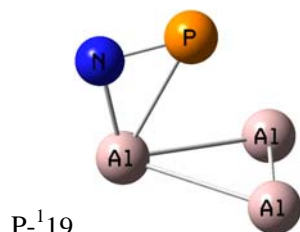Al,0,-1.0445482233,0.2290447869,0.

P-^{1}18

Al,0,-1.7594489538,0.0138519308,0.
Al,0,0.8065499885,-0.0310604769,0.
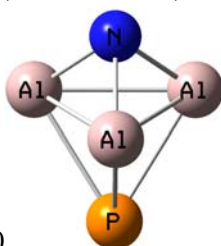N,0,2.4775746687,-0.2655669865,0.
P,0,-3.9582058487,0.0128029642,0.
Al,0,4.1843144752,0.0981349984,0.

P-^{1}19

N,0,-0.292971482,2.0412615912,0.

Al,0,-1.3390077744,0.4971493299,0.
Al,0,0.1646817792,-1.5063344601,-1.2904829272
P,0,1.0651468895,1.2351089854,0.
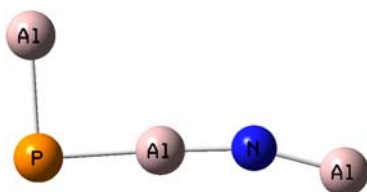Al,0,0.1646817792,-1.5063344601,1.2904829272

P-[1]20

Al,0,0.0000000025,1.4770225636,-0.3371753248
Al,0,1.2791390608,-0.7385112839,-0.3371753248
N,0,0.,0.,-1.518586184
Al,0,-1.2791390633,-0.7385112796,-0.3371753248
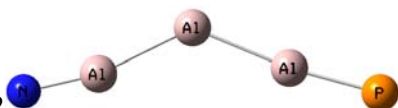P,0,0.,0.,1.6015023604
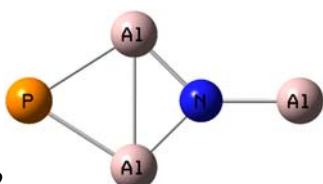
P-[3]02

Al,0,1.2923485922,0.,0.3295086435
Al,0,0.,0.,-2.8688430494
N,0,0.,0.,-0.9579268018
P,0,0.,0.,2.3326095542
Al,0,-1.2923485922,0.,0.3295086435

P-[3]21

Al,0,-1.35215413,-2.4624832534,-0.0167684141
N,0,1.5891147762,0.9605050537,-0.0703756217
Al,0,2.9433003596,1.9822503254,-0.0917561702
P,0,-2.1043016137,-0.3604762722,-0.0043098249
Al,0,-0.016586272,0.3862058765,-0.0413894291

P-[3]22

N,0,-0.3892269894,-0.66556622,-4.7218654388
Al,0,-0.1498646964,-0.2563282986,-2.939916172
Al,0,0.4448974737,0.7614672322,-0.7213729653
Al,0,-0.004432331,-0.0043319552,1.6355091022

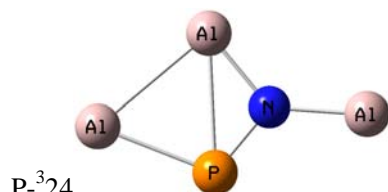P,0,-0.2665015169,-0.4532366185,3.835069034

P-^{3}23
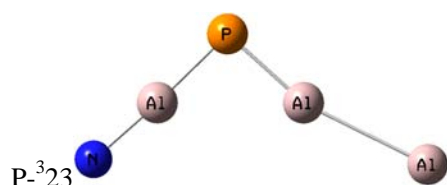
N,0,3.3605994191,-1.711415829,0.
Al,0,2.161959992,-0.2707576658,0.
Al,0,-3.9321917028,-0.6868550195,0.
P,0,0.8655588649,1.4531732155,0.
Al,0,-1.0206002932,0.2249202888,0.

P-^{3}24

N,0,0.8125705199,0.1736123555,0.
Al,0,-2.5420425774,-0.3793866056,0.
Al,0,-0.4355342425,1.5895503141,0.
Al,0,2.7670018009,0.1510915312,0.
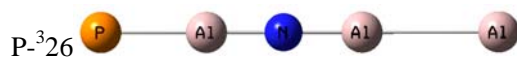P,0,-0.1812448908,-1.1867244851,0.

P-^{3}25

Al,0,-1.7855340264,-0.0192885263,0.
Al,0,0.7965133349,-0.0371779229,0.
N,0,2.4924372762,-0.0493386645,0.
P,0,-3.9450565925,-0.0045324941,0.
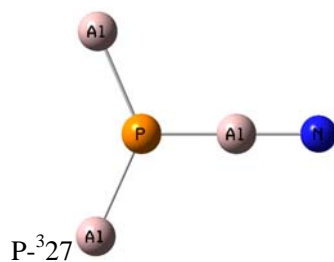Al,0,4.1924243378,-0.0614999622,0.

P-^{3}26

Al,0,0.,0.,4.6865039012
Al,0,0.,0.,1.690042725
N,0,0.,0.,-0.027757279
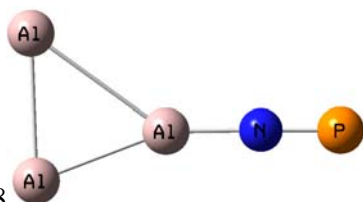P,0,0.,0.,-4.0294889215
Al,0,0.,0.,-1.7161748256

P-^{3}27

Al,0,0.,2.32917343,1.5125869765

Al,0,0.,-2.32917343,1.5125869765
N,0,0.,0.,-3.5330111927
Al,0,0.,0.,-1.6638359666
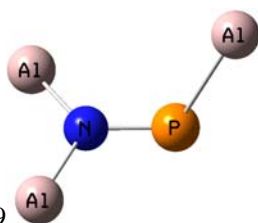P,0,0.,0.,0.4949515963

P-³28

Al,0,0.0483749803,1.5761068708,-2.6636185113
Al,0,0.0029500002,-0.0982013538,0.044932496
N,0,0.0011433424,0.057347384,1.8472620446
P,0,-0.0009476626,0.1647497251,3.3662146814
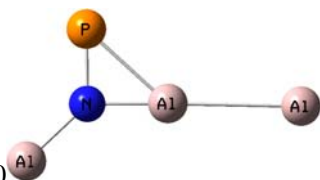Al,0,0.0138407596,-1.2304887761,-2.3475189206

P-³29

   Al,0,2.4413741809,1.5118802922,-0.2462369202
N,0,-0.5307669992,-0.4749123453,0.1699506321
Al,0,-2.1790629792,0.4166899314,-0.4181680925
Al,0,-0.240932149,-2.4062523043,-0.0390745232
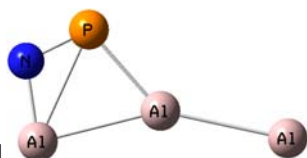P,0,0.5369126964,0.3839133061,1.1079019638

P-³30

   Al,0,-0.8191464666,-2.7644790619,0.
Al,0,-1.1172636118,3.6067788464,0.
P,0,1.8084119657,-0.7273856575,0.
N,0,0.1342407612,-1.1029641381,0.
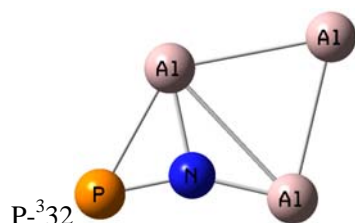Al,0,-0.3191866485,0.678189011,0.

P-³31

Al,0,-0.161532449,3.7029896694,0.
Al,0,1.5546878243,-1.6817882671,0.
N,0,-0.1162677967,-2.4677271665,0.
Al,0,0.0809621899,0.7667050239,0.
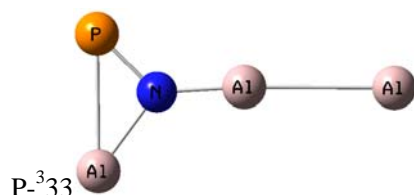P,0,-1.2074551685,-1.3134717898,0.

P-³32

Al,0,-0.1068577424,-1.4006539092,0.
Al,0,0.5276823562,1.7302495572,0.
N,0,-0.7677139334,0.4331709399,0.
P,0,-2.3466598828,-0.0945906521,0.
Al,0,2.6080658523,-0.3472487558,0.

P-³33

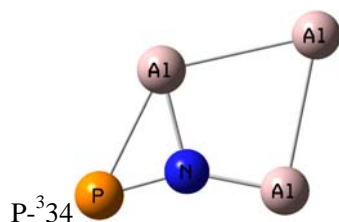N,0,-0.5335542017,0.6499241041,0.
Al,0,2.9179295672,-2.7526030569,0.
Al,0,0.7877965277,-0.5517262384,0.
Al,0,-2.5148626926,0.3715057119,0.
P,0,-0.5399172006,2.3536214794,0.

P-³34

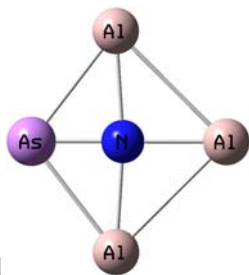N,0,-0.4816994193,0.8237776064,-0.271457917
Al,0,0.6923487312,1.6511310356,0.8677805908
Al,0,1.8466811463,-0.9643476918,1.5690929522
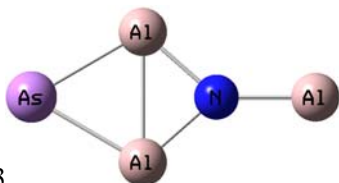P,0,-1.7295191196,0.814894999,-1.3748155628
Al,0,-0.3216221586,-1.1151107891,-0.3690433933
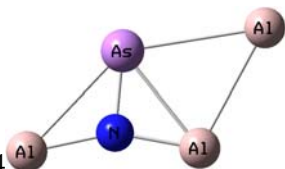
SI2-2-3: NAsAl$_3^+$

As-^{1}01

Al,0,0.,-2.1718648389,-0.0797519279
Al,0,0.,0.,2.0758188147
Al,0,0.,2.1718648389,-0.0797519279
N,0,0.,0.,0.0662578978
As,0,0.,0.,-1.7091420967

As-^{1}03

Al,0,-0.055167074,0.3392310084,-1.222185017
Al,0,0.0502369652,-2.8877476897,0.
N,0,-0.1228960436,-1.0358070272,0.
As,0,0.0624822469,2.4133289202,0.
Al,0,-0.055167074,0.3392310084,1.222185017

As-^{1}04

N,0,0.971253167,0.3534496178,0.
Al,0,-2.963319751,-0.3250904711,0.
Al,0,-0.5635122881,1.4648826974,0.
Al,0,2.9273041746,0.0425549026,0.
As,0,0.0490253074,-1.1876536367,0.
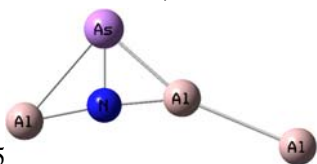
As-^{1}05

Al,0,-0.6042763615,-2.8708248688,0.
Al,0,-1.2286105722,3.6159993887,0.
As,0,1.6747693959,-0.9639400199,0.
N,0,-0.1567820461,-0.9776203155,0.
Al,0,0.001955584,0.8865248156,0.

As-^{1}06

Al,0,1.5898672936,-0.1725984625,0.
N,0,0.0317807245,0.7958203027,0.
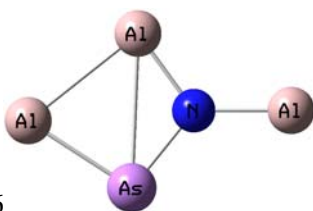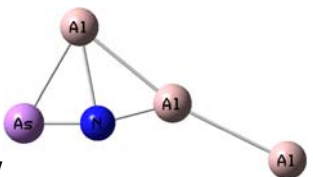Al,0,0.0566968588,-2.3760123843,0.
As,0,-1.3756805028,-0.5016666157,0.
Al,0,-0.1120046941,2.6707191098,0.

As-^{1}07

N,0,-0.0270882416,0.898324206,0.
Al,0,2.7984771907,-2.6290276216,0.
Al,0,0.3783544997,-0.8638780161,0.
Al,0,-2.2112653592,0.238986962,0.
As,0,-0.8210860895,2.4263164696,0.
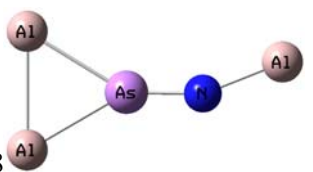
As-^{1}08

Al,0,0.,1.2233641885,2.272354875
N,0,0.,0.2989671354,-1.6630537165
Al,0,0.,-1.3637822422,2.0601390341
Al,0,0.,-0.251017981,-3.4572540434
As,0,0.,0.1374488993,0.002729851
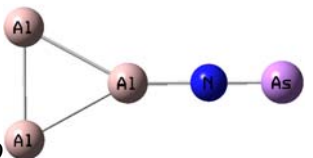
As-^{1}09

Al,0,0.,1.258692049,2.3790069156
Al,0,0.,0.,0.0652321316
N,0,0.,0.,-1.7500808425
As,0,0.,0.,-3.3897967503
Al,0,0.,-1.258692049,2.3790069156

As-^{1}10

Al,0,0.0591394542,3.9217409676,0.
Al,0,1.4112169715,-1.4630472266,0.
N,0,0.0315516882,-2.7054835421,0.
Al,0,-0.0457894695,0.8651774892,0.
As,0,-1.3057240444,-1.6116802181,0.

As-[1]11

N,0,0.,0.,-5.0019382835
Al,0,0.,0.,-3.2514084532
Al,0,0.,0.,-0.6898951902
Al,0,0.,0.,1.8645632797
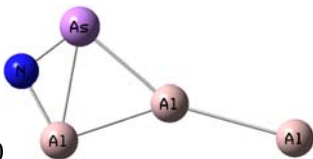As,0,0.,0.,4.1479642971

As-[1]12
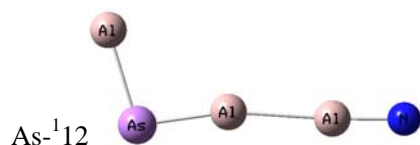
N,0,4.4608630162,0.4215902904,0.
Al,0,2.7254152656,0.0803851778,0.
Al,0,0.1929710254,-0.266872946,0.
As,0,-1.9401474483,-1.0259227633,0.
Al,0,-3.0997498488,1.1144851511,0.

As-[1]13

Al,0,0.,0.,4.7033955676
Al,0,0.,0.,1.708323355
N,0,0.,0.,-0.0119532538
As,0,0.,0.,-4.0879294676
Al,0,0.,0.,-1.7087106012

As-[1]14
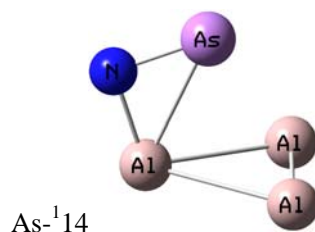
N,0,-0.3631013453,2.0686596492,0.
Al,0,-1.3430514832,0.5040850425,0.
Al,0,0.1572030087,-1.5204940948,-1.2877869185
As,0,1.1504422911,1.2263753778,0.
Al,0,0.1572030087,-1.5204940948,1.2877869185
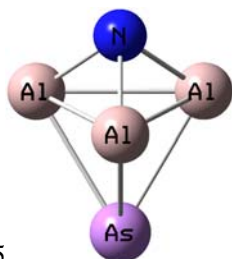
As-^{1}15

Al,0,0.0000000025,1.4951681022,-0.3706197469
Al,0,1.2948535582,-0.7475840533,-0.3706197469
N,0,0.,0.,-1.5218061491
Al,0,-1.2948535607,-0.7475840489,-0.3706197469
As,0,0.,0.,1.7052687595

As-^{3}02

Al,0,1.310396249,0.,-0.2623730707
Al,0,0.,0.,-3.4402631522
N,0,0.,0.,-1.5294251848
As,0,0.,0.,1.8635002283
Al,0,-1.310396249,0.,-0.2623730707
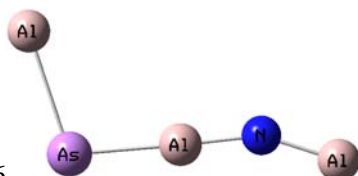
As-^{3}16

Al,0,0.5486088143,-0.6929972887,3.3069876177
N,0,0.3461084908,-0.4372008605,-2.0393126311
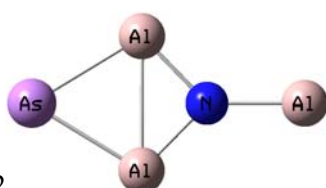Al,0,0.3991442683,-0.5041951359,-3.7466082159
As,0,-0.7665615989,0.9683131145,1.590531144
Al,0,-0.1394446046,0.1761450607,-0.5186115147
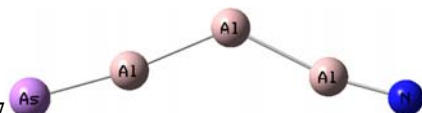
As-^{3}17

N,0,0.7506107294,0.1734875247,-5.6633047984
Al,0,0.2426119186,0.0469119572,-3.9002381132
Al,0,-0.8954580081,-0.2260446227,-1.6838324123
Al,0,-0.0000802906,-0.0047999712,0.6645974406
As,0,0.5572138507,0.136308602,2.9585657833

As-³18

N,0,1.2587037126,4.8122172619,0.0958929361
Al,0,0.6209828942,3.1276197135,0.018826905
Al,0,0.0793826638,0.6478869623,-0.0426831448
As,0,-0.9353722635,-1.3783532252,-0.1660997411
Al,0,1.0783439929,-2.7199707124,0.0940630448

As-³19

N,0,0.8497535812,0.2094377359,0.
Al,0,-2.5804825757,-0.3058827008,0.
Al,0,-0.4405029346,1.5408826281,0.
Al,0,2.7797573156,0.2323293685,0.
As,0,-0.1877747766,-1.3286239218,0.

As-³20

Al,0,0.,0.,4.7018377121
Al,0,0.,0.,1.7113582484
N,0,0.,0.,-0.005377643
As,0,0.,0.,-4.1086897673
Al,0,0.,0.,-1.6960029502

As-³21

Al,0,0.,1.2910969829,2.4376497674
Al,0,0.,0.,0.0015865882
N,0,0.,0.,-1.7623539062
As,0,0.,0.,-3.4311638468
Al,0,0.,-1.2910969829,2.4376497674

As-³22

Al,0,-0.848398138,-2.7286979165,0.
Al,0,-1.1446947483,3.6248273509,0.
As,0,1.9513662772,-0.8287947482,0.

N,0,0.0749079462,-1.0678034409,0.
Al,0,-0.3461253371,0.6906077546,0.
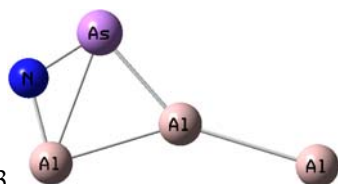
As-[3]23

Al,0,-0.0401188757,3.7234913413,0.
Al,0,1.5478017311,-1.5561082033,0.
N,0,0.0013987035,-2.5212653379,0.
Al,0,-0.0226974679,0.7558676375,0.
As,0,-1.335989491,-1.3952779676,0.
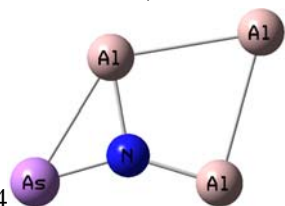
As-[3]24

N,0,-0.4471775345,0.7665123833,-0.2478157704
Al,0,0.6929877117,1.6483153611,0.8686642654
Al,0,1.8812723029,-0.9763851924,1.5971470615
As,0,-1.8360238974,0.8867218974,-1.4611478137
Al,0,-0.2848694028,-1.1148192893,-0.3352910728

As-[3]25

Al,0,0.5529003416,1.7907649585,-0.1440531178
Al,0,-0.5166447443,0.,-2.6482432234
Al,0,0.5529003416,-1.7907649585,-0.1440531178
N,0,0.1229776488,0.,-0.7708446209
As,0,-0.5999475877,0.,1.2259270798

SI3-1 The details of MD simulations.

General parameters:

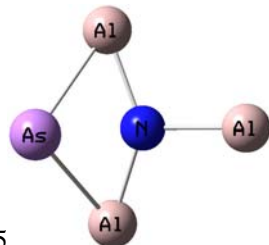|		
Max. points for each Traj.	=	4000
Total Number of Trajectories	=	1
Random Number Generator Seed	=	398465
Trajectory Step Size	=	0.500 sqrt(amu)*bohr

Sampling parameters:

Vib Energy Sampling Option	= Thermal sampling	
TS Sampling direction	=	Forward
Vib Sampling Temperature	=	373.0 K
Rot Energy Sampling Option	= Thermal distribution (symmetric top)	
Rot Sampling Temperature	=	373.0 K
Start point scaling criteria	=	1.000D-05 Hartree

Integration parameters:

Correction Scheme	= Fifth order polynomial fit
Project trans/rot in grad.	= True
Project in prediction step	= True
Project in correction step	= True
Integration Scheme	= Bulirsch-Stoer method
Integration Step Size	= 2.000D-01 femtosec
Truncation Error Criteria	= 1.000D-08 bohr
Energy Error Criteria	= 1.000D-04 Hartree
Hessian evaluation	= Full Hessian always

SI3-2 Potential energy of three designed pptNs of the $NXAl_3^+$ (X=N, P, As). (a) $N_2Al_3^+$, (b) $NPAl_3^+$, and (c) $NAsAl_3^+$ along the MD trajectory at B3LYP/6-31G(d) level, respectively. Born-Oppenheimer molecular dynamics simulation is performed for 14ps at 373K. Potential energy (in au) versus time (in ps).

373k

(a) $N_2Al_3^+$

373k

(b) $NPAl_3^+$

373k

(c) $NAsAl_3^+$