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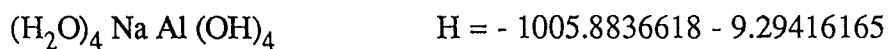
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Supplementary materials

The positions of atoms in each cluster are described in the orthogonal coordinates. The position is given in atomic units (1 a.u. = 0.0529 nm).

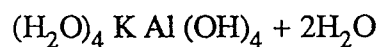


	x	y	z
Al	0.6598902198E+00	0.7205926707E-01	0.1196049583E+00
O	0.5564757540E+00	-0.1053313332E+01	0.3368960463E+01
O	0.4009302452E+01	-0.3554572200E+00	-0.3337473541E+00
O	-0.1620289409E+00	0.3282145902E+01	0.5683073766E+00
O	-0.7771868340E+00	-0.1792156829E+01	-0.2154967446E+01
O	0.8105934149E+01	0.8100978766E+00	0.2180769589E+01
O	0.4240803158E+01	-0.2204119722E+00	0.7436139241E+01
O	0.4292913462E+01	-0.4202265731E+01	0.3804376169E+01
O	0.3732792065E+01	0.3580896307E+01	0.3613368089E+01
H	-0.1049065451E+01	-0.7160836639E+00	0.4198768156E+01
H	0.4247141051E+01	-0.1808892006E+01	-0.1443467035E+01
H	-0.7164391445E+00	0.4263829434E+01	-0.8813573609E+00
H	-0.2584308191E+01	-0.2073313813E+01	-0.2178308408E+01
H	0.9499914445E+01	-0.3863403084E+00	0.2103187419E+01
H	0.7023432696E+01	0.4948232064E+00	0.6513235460E+00
H	0.5158643853E+01	0.1290750131E+01	0.7952623247E+01
H	0.2619102673E+01	0.4245149233E+00	0.6796221007E+01
H	0.2494732390E+01	-0.3612435858E+01	0.3674472962E+01
H	0.4559852733E+01	-0.4375657946E+01	0.5620643437E+01
H	0.2273650851E+01	0.3956807018E+01	0.2427857792E+01
H	0.5223604658E+01	0.4331026059E+01	0.2827731792E+01
Li	0.4743476124E+01	-0.3141685192E+00	0.3532559025E+01



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	x	y	z
Al	0.2589837135E+00	-0.3496793244E-01	-0.1749869532E+00
O	0.4454020093E+00	-0.1117042596E+01	0.3079519824E+01
O	0.3560987083E+01	-0.2369586675E+00	-0.8435639616E+00
O	-0.5235895487E+00	0.3212506078E+01	0.2394191820E+00
O	-0.1775421594E+01	-0.1527293539E+01	-0.2268014837E+01
O	0.9050722471E+01	0.5536631656E+00	0.2468148724E+01
O	0.5095796319E+01	0.5832101343E-01	0.7733474162E+01
O	0.4456845921E+01	-0.3985478297E+01	0.3722500145E+01
O	0.3634392234E+01	0.4561345128E+01	0.2406103596E+01
H	-0.1015068747E+01	-0.6447394743E+00	0.4089182487E+01
H	0.3954369660E+01	-0.1533267736E+01	-0.2087270579E+01
H	-0.1303326131E+01	0.4058343717E+01	-0.1191414411E+01
H	-0.2396086411E+01	-0.3212015815E+01	-0.1914495828E+01
H	0.1058880783E+02	0.2874435666E+00	0.3437718644E+01
H	0.9025160408E+01	-0.7886683348E+00	0.1199635783E+01
H	0.6362837205E+01	0.1129361027E+01	0.8527372128E+01
H	0.3473816328E+01	0.8213052145E+00	0.8165521934E+01
H	0.2658518728E+01	-0.3379317551E+01	0.3600090973E+01
H	0.4742137069E+01	-0.4236588819E+01	0.5522417297E+01
H	0.4769469917E+01	0.4824394365E+01	0.9745391635E+00
H	0.1928913806E+01	0.4306414528E+01	0.1518415823E+01
Na	0.4783148689E+01	0.4089262703E+00	0.3188321074E+01

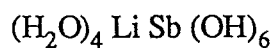


$$\text{H} = -1594.13622007 - 11.8603177$$

	x	y	z
Al	0.1952281314E+00	0.3183259046E-01	-0.3280547891E+00
O	0.8644775117E+00	-0.3592733208E+00	0.2936858407E+01
O	0.3482975488E+01	-0.9544189452E-01	-0.1486126241E+01
O	-0.8285645855E+00	0.3151001335E+01	-0.9060458606E+00
O	-0.1210657174E+01	-0.2407499274E+01	-0.2053823299E+01

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O	0.1116042215E+02	0.7986797718E+00	0.3217816272E+01
O	0.6102630973E+01	0.4788259719E+00	0.9298547147E+01
O	0.5649070545E+01	-0.3991882401E+01	0.6465005492E+00
O	0.8042961611E+01	-0.4123252596E+01	0.1030615613E+02
O	0.4782774662E+01	0.4245659115E+01	0.5846618987E+00
O	0.7196941847E+01	0.5866600220E+01	0.9758986649E+01
H	-0.6181264472E+00	-0.2114145255E+00	0.4009027585E+01
H	0.3454576638E+01	-0.2233636228E+00	-0.3321755463E+01
H	-0.2319579907E+01	0.3353354217E+01	-0.1956468234E+01
H	-0.3002625492E+01	-0.2763616427E+01	-0.1922121077E+01
H	0.1220899251E+02	0.1985451172E+01	0.4154230486E+01
H	0.1160880810E+02	0.1065142300E+01	0.1451963917E+01
H	0.6855102941E+01	-0.1176816400E+01	0.9821304871E+01
H	0.4447914699E+01	0.5209990803E+00	0.1010754277E+02
H	0.4376503268E+01	-0.5309496590E+01	0.8406640979E+00
H	0.4749622544E+01	-0.2646688608E+01	-0.3775740885E+00
H	0.7626810461E+01	-0.4979837651E+01	0.1188391665E+02
H	0.7752313404E+01	-0.5361250231E+01	0.8972020308E+01
H	0.3118072250E+01	0.5057207816E+01	0.5864912355E+00
H	0.4430369117E+01	0.2735839010E+01	-0.5198568090E+00
H	0.6676980167E+01	0.6210786094E+01	0.8027683742E+01
H	0.7054652812E+01	0.4019121226E+01	0.9909007443E+01
K	0.5749205739E+01	0.2284010392E+00	0.3846364000E+01

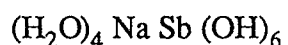


$$H = -766.14017619 - 8.9366839$$

	x	y	z
Sb	0.1374855527E-01	0.1573563145E+00	0.2450605983E+00
O	-0.2497840046E+00	-0.3516291261E+00	0.3930406929E+01
O	0.2241665581E+00	0.1014292289E+01	-0.3370254142E+01
O	0.3716131551E+01	-0.2203919723E+00	0.6793069730E+00
O	-0.3653807725E+01	0.4860268804E+00	0.2955690286E+00
O	0.7717834576E+00	0.3759320688E+01	0.8690386070E+00

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O	-0.2131626235E-01	-0.3427906920E+01	-0.6351308321E+00
O	0.3975004593E+01	0.7263756128E+01	0.4513386442E+01
O	0.7034639530E+01	0.3664987407E+01	0.4351550536E+01
O	0.5312036699E+01	0.3181645326E+01	-0.2406050083E+01
O	0.2967021552E+01	0.2509346109E+01	0.6356884659E+01
H	-0.1967201422E+01	0.1524071501E+00	0.4399444198E+01
H	0.2273732354E+00	-0.6034885026E+00	-0.4265417962E+01
H	0.4049343278E+01	-0.2011369947E+01	0.9933505747E+00
H	-0.4191086714E+01	0.8859623760E+00	-0.1423802861E+01
H	0.4101019529E-02	0.4754457734E+01	-0.4842288255E+00
H	-0.1594340188E+01	-0.4135451955E+01	0.2284604182E-01
H	0.5654892095E+01	0.6483371451E+01	0.4912203274E+01
H	0.3936942153E+01	0.8954780851E+01	0.5231296515E+01
H	0.5552982514E+01	0.2790987497E+01	0.5376696578E+01
H	0.8670259741E+01	0.3012497909E+01	0.4890755449E+01
H	0.5147468505E+01	0.1440837006E+01	-0.1683339089E+01
H	0.3770574397E+01	0.3230936339E+01	-0.3440412986E+01
H	0.2432769008E+01	0.4256811935E+01	0.5962623961E+01
H	0.1747132138E+01	0.1345184267E+01	0.5406797821E+01
Li	0.4544054050E+01	0.3999600757E+01	0.1269762755E+01



$$\text{H} = -920.13019391 - 9.81262388$$

	x	y	z
Sb	-0.5807791500E-01	0.1245159210E+00	0.1963143865E+00
O	-0.2442016439E+00	-0.3587345800E+00	0.3892191377E+01
O	0.6500561678E-01	0.9990376699E+00	-0.3419551891E+01
O	0.3655133758E+01	-0.1752838545E+00	0.6049996373E+00
O	-0.3752806322E+01	0.2091288558E+00	0.3277557232E+00
O	0.4284722151E+00	0.3769818514E+01	0.7783027589E+00
O	-0.9033417633E-02	-0.3466423060E+01	-0.6471516346E+00
O	0.4025898506E+01	0.7304898418E+01	0.4755517250E+01
O	0.7247232356E+01	0.3807484075E+01	0.4794511764E+01

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O	0.5349071029E+01	0.3040242426E+01	-0.2673382235E+01
O	0.2996108833E+01	0.2466011391E+01	0.6267016329E+01
H	-0.1949116443E+01	0.1656839957E+00	0.4379791347E+01
H	0.1972422989E+00	-0.6085620966E+00	-0.4323483684E+01
H	0.4025209318E+01	-0.1970492801E+01	0.8432095470E+00
H	-0.4351799503E+01	0.8340514127E+00	-0.1303818359E+01
H	-0.1799171102E+00	0.4636145237E+01	-0.7340133821E+00
H	-0.1629255610E+01	-0.4147848458E+01	-0.8208620943E-01
H	0.5676341169E+01	0.6540390522E+01	0.5311893850E+01
H	0.3845965987E+01	0.8946804106E+01	0.5558293322E+01
H	0.5706648562E+01	0.2810123735E+01	0.5558574563E+01
H	0.8828413045E+01	0.3176660192E+01	0.5485998182E+01
H	0.5058523535E+01	0.1415209764E+01	-0.1740008427E+01
H	0.3846571742E+01	0.3073883603E+01	-0.3753258481E+01
H	0.2466006812E+01	0.4228645031E+01	0.5959783427E+01
H	0.1775184756E+01	0.1328037140E+01	0.5282038224E+01
Na	0.4703833600E+01	0.4492539625E+01	0.1306810687E+01

(H₂O)₇ K Sb (OH)₆

H = - 1584.08663828 - 13.2483453

	x	y	z
Sb	-0.4338799208E+01	-0.6092343631E+00	-0.2452572891E+00
O	-0.2114800233E+01	0.2418782944E+00	0.2683768735E+01
O	-0.6210287272E+01	-0.2011196472E+01	-0.3079533110E+01
O	-0.2087235179E+01	-0.3506008906E+01	-0.7628007874E+00
O	-0.6323106377E+01	0.2487805723E+01	-0.2207640167E+00
O	-0.1892145552E+01	0.1455105660E+01	-0.2214786697E+01
O	-0.6459211837E+01	-0.2113733832E+01	0.2373088790E+01
O	0.4391576814E+01	0.4394916507E+01	0.4211552771E+00
O	0.5637798520E+01	-0.2191382972E+01	0.4012561507E+01
O	0.1536127945E+01	0.3960665584E-01	-0.5275737099E+01
O	0.6124948464E+01	-0.8361182847E+00	-0.3686865995E+01
O	0.2040960234E+00	0.4520912234E+01	0.2890771148E+01

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O	0.1571157821E+01	-0.5395321903E+01	0.2166832064E+01
O	0.7980838343E+01	0.8737428017E+00	0.8177605488E+00
H	-0.2924244075E+01	-0.5475663255E+00	0.4149227852E+01
H	-0.7364618335E+01	-0.6996998917E+00	-0.3675904173E+01
H	-0.2604023149E+01	-0.4324234061E+01	-0.2339715933E+01
H	-0.7474776824E+01	0.2377975040E+01	0.1217057698E+01
H	-0.2470083882E+01	0.3211559955E+01	-0.2134189227E+01
H	-0.7266675516E+01	-0.3617268364E+01	0.1672748480E+01
H	0.4612625475E+01	0.5892814892E+01	-0.6218526900E+00
H	0.2779878111E+01	0.4629478180E+01	0.1456154850E+01
H	0.5797368320E+01	-0.3917231485E+01	0.3385994485E+01
H	0.6818497715E+01	-0.1138759995E+01	0.2946245093E+01
H	0.9147126726E+00	-0.4894475932E+00	-0.6916102896E+01
H	0.2662169393E-01	0.6694112431E+00	-0.4242003928E+01
H	0.7216336385E+01	-0.1613069373E+01	-0.4941971500E+01
H	0.4486832610E+01	-0.3861873679E+00	-0.4563689750E+01
H	0.3806674947E+00	0.5064552074E+01	0.4639446373E+01
H	-0.8093862225E+00	0.2874220396E+01	0.2926436149E+01
H	-0.5115329351E-01	-0.4986567110E+01	0.1308152681E+01
H	0.1518917376E+01	-0.4562202769E+01	0.3808209334E+01
H	0.6961424269E+01	0.2456846584E+01	0.9250784532E+00
H	0.7638727640E+01	0.2945572274E+00	-0.9365046455E+00
K	0.2575508275E+01	-0.6737111739E+00	0.1256488001E+00

Al(OH)₄⁻ H = - 541.85796149 - 4.68769308

	x	y	z
Al	0.2849295201E-01	0.3101622309E-01	-0.2224445948E-01
O	0.3023965462E+00	0.2996234512E-02	0.3343613501E+01
O	0.3170232969E+01	0.1861775037E+00	-0.1260754384E+01
O	-0.1701871819E+01	0.2682292286E+01	-0.1202819072E+01
O	-0.1630415624E+01	-0.2758593124E+01	-0.9587361892E+00
H	-0.1343474001E+01	-0.1005383355E+00	0.4142234705E+01

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H	0.4217052847E+01	-0.1083890433E+01	-0.4543368939E+00
H	-0.8422783297E+00	0.4250815826E+01	-0.8065012663E+00
H	-0.1799288880E+01	-0.2834803668E+01	-0.2784953975E+01

Sb (OH)₆⁻ H = - 456.09147934 - 5.21426639

	x	y	z
Sb	-0.8233303726E-03	-0.1494579913E-03	0.7057489203E-03
O	-0.5861745883E-01	0.1663699754E+00	0.3733746334E+01
O	0.5762369246E-01	-0.1739574761E+00	-0.3730056357E+01
O	0.3731366122E+01	0.5882092346E-01	0.1635114826E+00
O	-0.3732226284E+01	-0.5760243168E-01	-0.1621533420E+00
O	-0.1614825825E+00	0.3731149902E+01	-0.5968655250E-01
O	0.1573496068E+00	-0.3729610587E+01	0.6077238033E-01
H	0.1708167104E+01	-0.6245532350E-01	0.4184443003E+01
H	-0.1706838781E+01	0.6447827273E-01	-0.4185360217E+01
H	0.4187295072E+01	-0.1707089152E+01	-0.6183629223E-01
H	-0.4185291941E+01	0.1709117553E+01	0.6117857104E-01
H	0.6445051576E-01	0.4182484122E+01	0.1707419548E+01
H	-0.5933580531E-01	-0.4174097903E+01	-0.1709856185E+01

Li (OH₂)₄⁺ H = - 309.84103196 - 3.7309348

	x	y	z
Li	-0.2112316449E-01	-0.3881868588E-01	-0.1486116531E-01
O	-0.1612266975E-02	-0.1256785132E+00	0.3602230218E+01
O	0.3420660354E+01	0.3417174538E-01	-0.1090300886E+01
O	-0.1648080044E+01	0.2900771845E+01	-0.1324849348E+01
O	-0.1875787233E+01	-0.2904910258E+01	-0.1196891296E+01
H	-0.1463579930E+01	0.4620740638E-01	0.4709345278E+01
H	0.4748027352E+01	-0.1184700693E+01	-0.7065073923E+00
H	-0.1243929683E+01	0.4653623813E+01	-0.9253398998E+00

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H	-0.1998446326E+01	-0.3525342826E+01	-0.2928406230E+01
H	0.1480210641E+01	-0.2728183007E-01	0.4693894308E+01
H	0.4159662038E+01	0.1239135278E+01	-0.2276747846E+01
H	-0.3222527400E+01	0.2937845213E+01	-0.2285492428E+01
H	-0.2544529522E+01	-0.4248078784E+01	-0.1256064191E+00

Na (OH₂)₄⁺ H = - 463.82552007 - 4.6101315

	x	y	z
Na	0.1560421029E+00	-0.9142469472E-01	-0.1074753880E-03
O	0.2623711196E-01	-0.1522459614E+00	0.4205866855E+01
O	0.4135074660E+01	0.1898828377E-01	-0.1297378312E+01
O	-0.1811340397E+01	0.3283322453E+01	-0.1495597289E+01
O	-0.2195983967E+01	-0.3289734089E+01	-0.1339824828E+01
H	-0.1476968488E+01	0.1005663678E+00	0.5240226012E+01
H	0.5460621272E+01	-0.1189913840E+01	-0.8966377446E+00
H	-0.1457009545E+01	0.5047910868E+01	-0.1104874466E+01
H	-0.2403372062E+01	-0.3954723983E+01	-0.3044735305E+01
H	0.1446881532E+01	-0.3155192091E-01	0.5372392505E+01
H	0.4906647340E+01	0.1234862747E+01	-0.2443249178E+01
H	-0.3384518628E+01	0.3298575231E+01	-0.2454754336E+01
H	-0.2895488223E+01	-0.4575200010E+01	-0.2237313918E+00

K (OH₂)₆⁺ H = - 1052.08917105 - 7.17266654

	x	y	z
K	-0.1722755878E-01	0.8590769653E-02	0.1618523751E-01
O	-0.8654397231E+00	0.1105424142E-01	0.5245836647E+01
O	0.9288952409E+00	-0.2383097139E-01	-0.5182852432E+01
O	0.5026093466E+01	-0.6455181874E+00	0.8299317661E-01
O	-0.5060149377E+01	0.7202759695E+00	-0.5082577303E-01
O	0.7213583286E+00	0.5152485713E+01	0.3017357638E-01

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O	-0.7914479891E+00	-0.5133311228E+01	-0.8967995675E-02
H	-0.9015838765E+00	0.1470804850E+01	0.6368236777E+01
H	-0.9156740849E+00	-0.1437877411E+01	0.6381976267E+01
H	0.8762388002E+00	0.1408849133E+01	-0.6339229906E+01
H	0.9038009468E+00	-0.1497317255E+01	-0.6288798381E+01
H	0.6303488245E+01	-0.8747969069E+00	0.1388772641E+01
H	0.5947158654E+01	-0.7403580299E+00	-0.1508504377E+01
H	-0.6009679507E+01	0.6757169098E+00	0.1525512986E+01
H	-0.6334435258E+01	0.8426150684E+00	-0.1373456585E+01
H	0.1158258270E+01	0.6231510127E+01	0.1456413825E+01
H	0.7953835748E+00	0.6273002853E+01	-0.1428187123E+01
H	-0.7417290825E+00	-0.6306296367E+01	0.1409184137E+01
H	-0.1180617438E+01	-0.6195361121E+01	-0.1462089951E+01

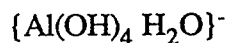
H₂O H = - 75.64949079 - 0.88425914

	x	y	z
O	0.2359967891E-02	0.1552767790E-02	-0.5552271138E-02
H	0.1839911497E+01	0.1373829403E-01	0.2221318441E-02
H	-0.4732939435E+00	0.1777154611E+01	0.2732617448E-02

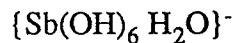
(H₂O)₂ H = - 151.31272857 - 1.76429372

	x	y	z
O	-0.1219230241E-01	0.1854396731E-02	-0.1807334490E-02
O	0.5193786860E+01	0.1010361101E-01	0.5494278828E-03
H	0.1856280253E+01	0.1906092046E-01	-0.2619640219E-04
H	-0.4802213360D+00	0.1777596762E+01	0.6614161548E-03
H	0.5790710745E+01	-0.9312259624E+00	0.1466456480E+01
H	0.5787367695E+01	-0.9306440189E+00	-0.1467054163E+01

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	x	y	z
Al	0.6671562138E-01	-0.3243663630E-01	0.4823929433E-01
O	0.1906187244E+00	-0.2200532074E+00	0.3468557968E+01
O	0.3220643695E+01	0.1958053251E+00	-0.1066218030E+01
O	-0.1618616877E+01	0.2686593378E+01	-0.9453400324E+00
O	-0.1618616877E+01	-0.2748282792E+01	-0.9845890270E+00
O	0.2278734914E+01	-0.2536877028E+01	0.7418844574E+01
H	-0.1535180429E+01	-0.5658611077E-01	0.4068730821E+01
H	0.4276225328E+01	-0.1107633575E+01	-0.3317415568E+00
H	-0.6366598812E+00	0.4210298039E+01	-0.7983607566E+00
H	-0.1826934774E+01	-0.2704604054E+01	-0.2806834877E+01
H	0.1557559171E+01	-0.1674713159E+01	0.5858861617E+01
H	0.9992960978E+00	-0.22255283346E+01	0.8700422756E+01



	x	y	z
Sb	0.1439944178E+00	0.1323149350E+00	-0.1470376405E+00
O	-0.2846488858E+00	0.1434301568E+00	0.3619032757E+01
O	-0.9160246865E-02	-0.3567757937E+00	-0.3843912246E+01
O	0.3844368517E+01	-0.1474847494E-01	-0.3057180717E-01
O	-0.3621460719E+01	-0.2373524314E+00	-0.1118080793E+00
O	0.2045921038E-01	0.3829930016E+01	-0.2907496048E-01
O	0.1123330705E+00	-0.3633547811E+01	-0.2163519101E+00
O	-0.2250856499E+01	-0.3263671773E+01	0.6447993177E+01
H	0.2115247207E+01	0.7154768061E-02	0.3880646055E+01
H	-0.1809669382E+01	0.2131948027E+00	-0.4183671536E+01
H	0.4173751246E+01	-0.1821907372E+01	-0.2387765029E+00
H	-0.3903371923E+01	0.2066776711E+01	0.5040982640E-02

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H	0.2159560722E+00	0.4173068357E+01	0.1777995581E+01
H	-0.6571409169E-01	-0.3922405076E+01	-0.2038877451E+01
H	-0.1103052811E+01	-0.2096628157E+01	0.5495981178E+01
H	-0.3929623399E+01	-0.2645706349E+01	0.5805252147E+01