Al_4^{2-}; From Aromaticity to Molecular Machines

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The electronic delocalization indices between various atomic basins in Al_4 complexes; $2*D2(A,B) = 2*D2(B,A)$ = Average Number of Electron Pairs Shared Between Atoms A and B; $DI(A,B) = DI(B,A)$ = Electron Delocalization Index. Average Number of Electrons Delocalized (Shared) Between Atoms A and B. Bond Index When Atoms A and B Connected by a Bond Path;
$\%Deloc(A,B) = 100 * (DI(A,B)/2)/N(A)$ = Percentage of Average Number of Electrons in Atom A That are Shared With Atom B;
$\%Deloc(B,A) = 100 * (DI(A,B)/2)/N(B)$ = Percentage of Average Number of Electrons in Atom B That are Shared With Atom A page S-15.

Molecule	$\lvert\mu_{zz}(\Omega)^{intra}\rvert$	$\lvert\mu_{zz}(\Omega\lvert\Omega')\rvert$
Al_4^{2-}	0.000	0.000
Al_4^{2-} (π)	0.000	0.000
Al_4^{2-} (σ)	0.000	0.000
$LiAl_4^-$	0.622	0.010
$LiAl_4^-$ (π)	0.041	0.070
$LiAl_4^-$ (σ)	0.581	0.003
Li_2Al_4	0.004	0.000
$Li_2Al_4^-$ (π)	0.002	0.000
$Li_2Al_4^-$ (σ)	0.002	0.000
$NaAl_4^-$	0.427	0.004
$NaAl_4^-$ (π)	0.005	0.000
$NaAl_4^-$ (σ)	0.422	0.004
Na_2Al_4	0.000	0.000
$Na_2Al_4^-$ (π)	0.000	0.000
$Na_2Al_4^-$ (σ)	0.000	0.000
KAl_4^-	0.347	0.008
KAl_4^- (π)	0.034	0.003
KAl_4^- (σ)	0.313	0.005
K_2Al_4	0.000	0.000
$K_2Al_4^-$ (π)	0.000	0.000
$K_2Al_4^-$ (σ)	0.000	0.000
$MgAl_4$	0.428	0.010
$MgAl_4$ (π)	0.273	0.032
$MgAl_4$ (σ)	0.701	0.022
$CaAl_4$	0.518	0.029
$CaAl_4$ (π)	0.018	0.014
$CaAl_4$ (σ)	0.536	0.015

a. Average values

Bond Length Variation (Å)

$y = 13.4026x^2 - 0.6875x - 5.6488$
$R^2 = 0.9875$

π-Isotropic Intra-Atomic Magnetizability (cgs-ppm)

Figure S-1

Bond Length Variation (Å)

$R^2 = 0.9958$

● Total Magnetizability
■ σ-Magnetizability

$R^2 = 0.9497$

Isotropic Intra-Atomic Magnetizability (cgs-ppm)
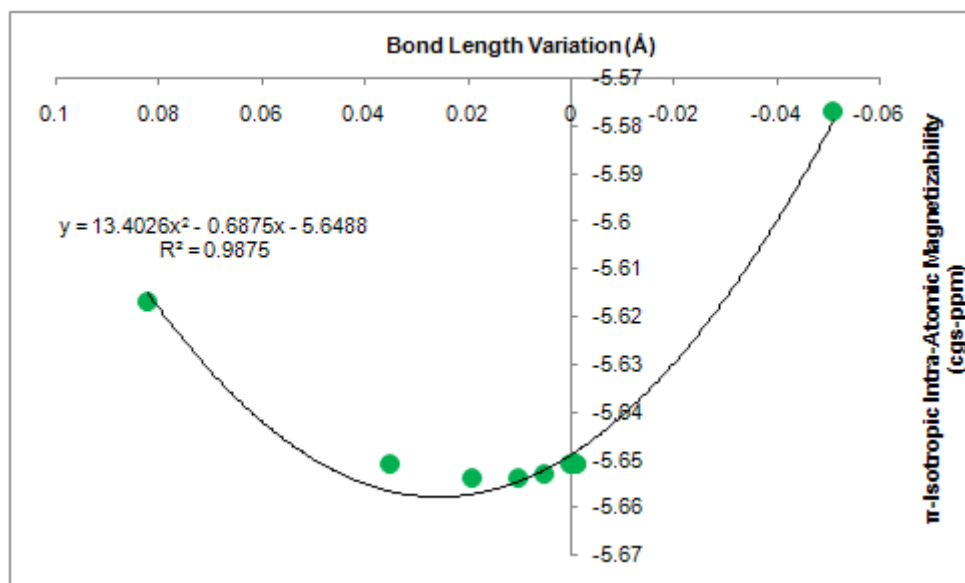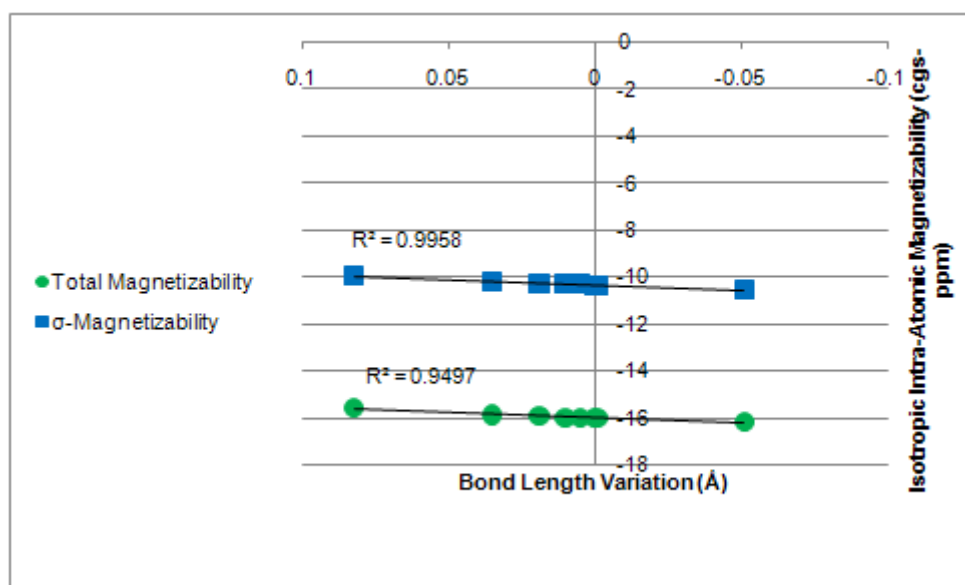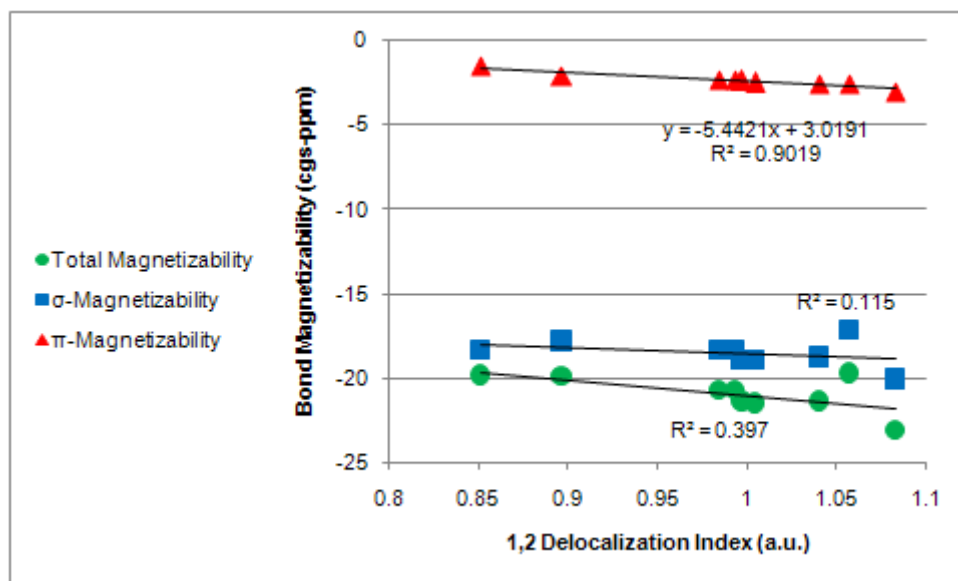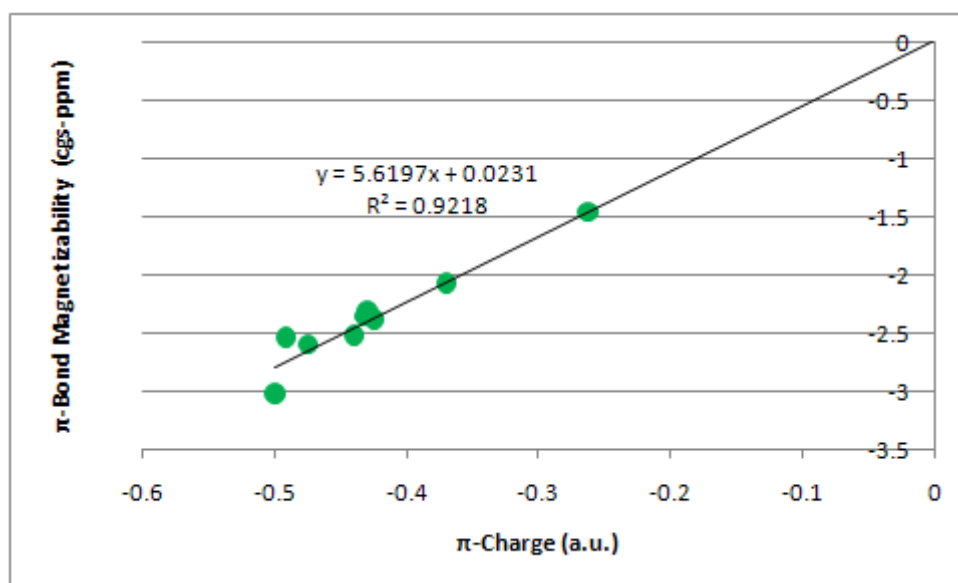
Figure S-2

Figure S-3

Figure S-4
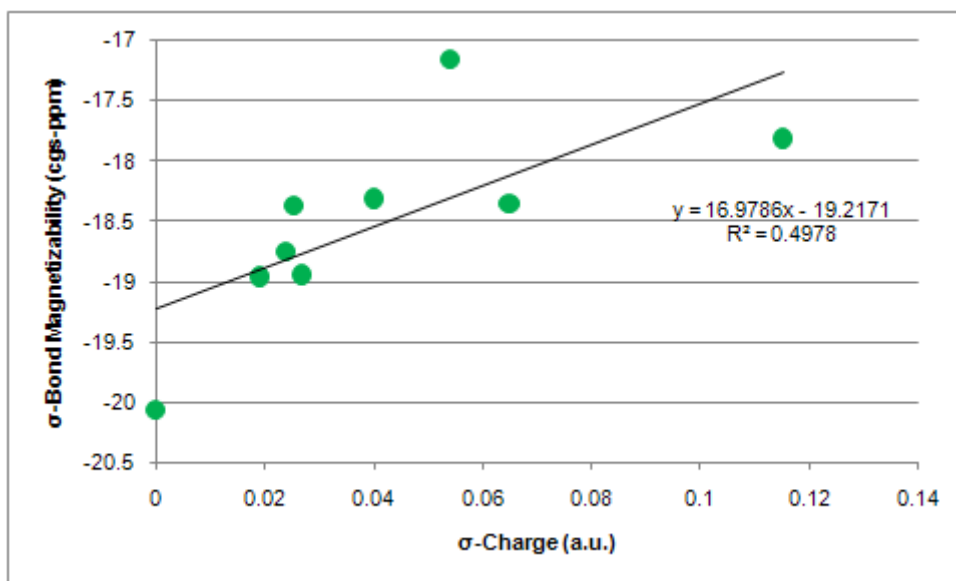
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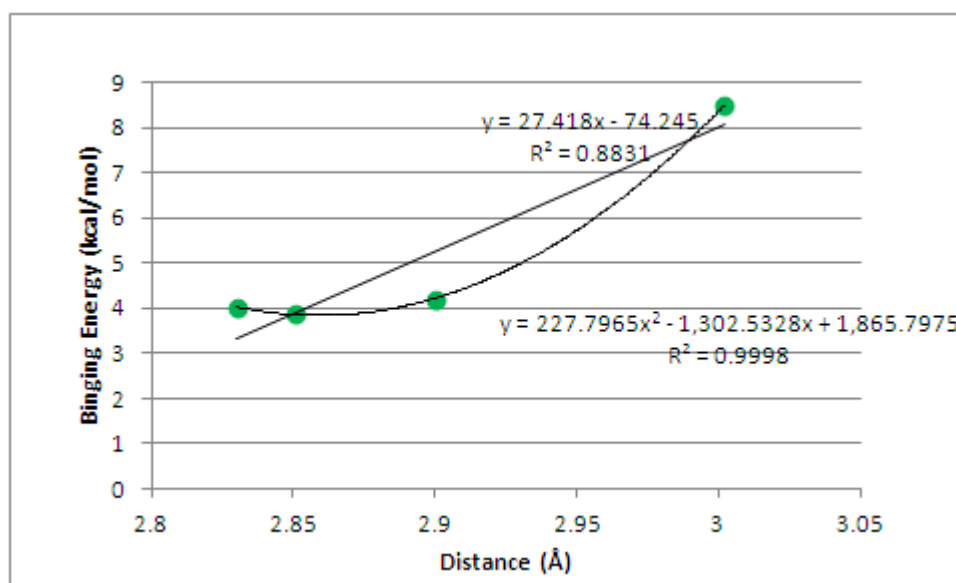
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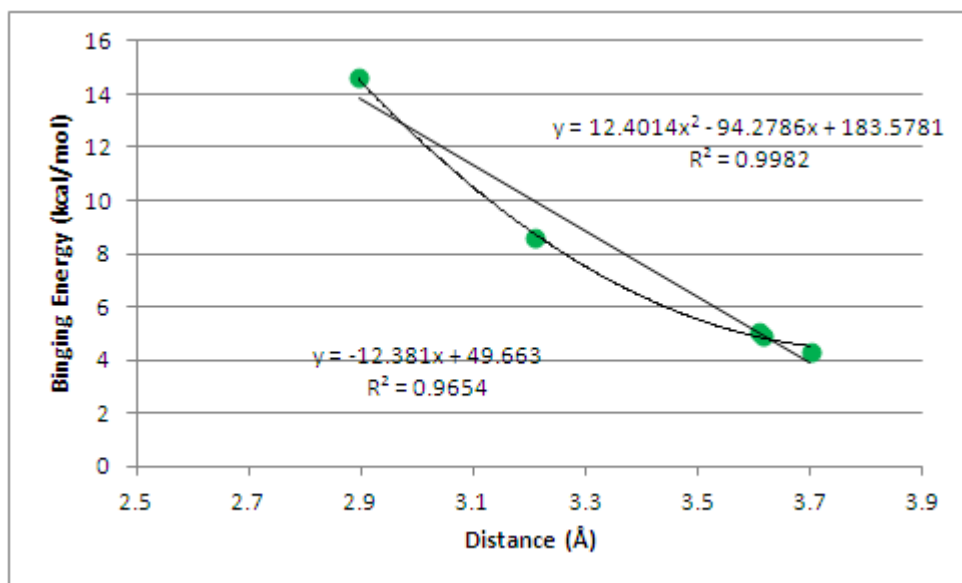
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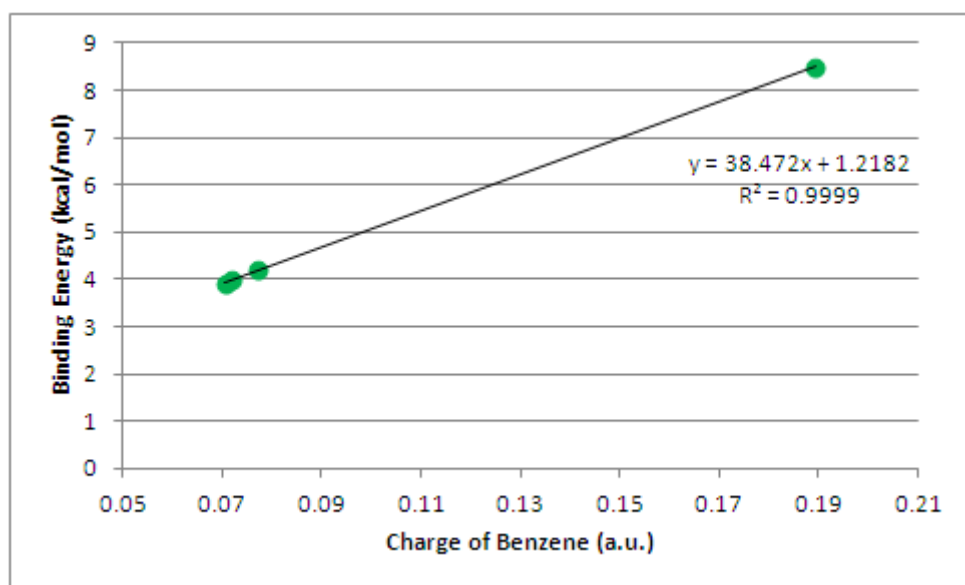
Figure S-8
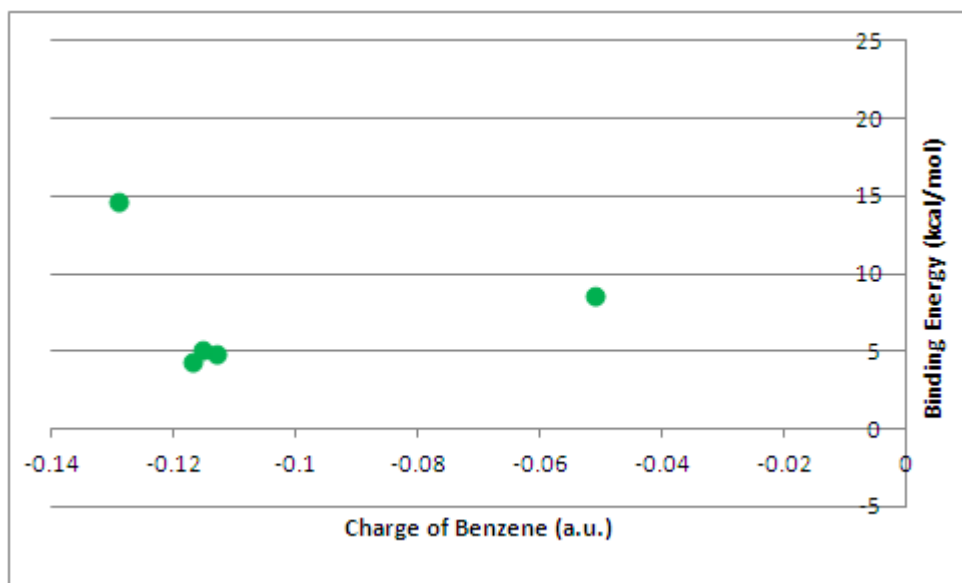
Figure S-9

$Al_4{}^{2-}$

13	0.000000000	1.812632218	0.000000000
13	1.812632218	0.000000000	0.000000000
13	-1.812632218	0.000000000	0.000000000
13	0.000000000	-1.812632218	0.000000000

$LiAl_4{}^-$

13	0.000000000	1.810325137	-0.120052009
13	-1.810325137	0.000000000	-0.120052009
13	1.810325137	0.000000000	-0.120052009
13	0.000000000	-1.810325137	-0.120052009
3	0.000000000	0.000000000	2.080896158

Li_2Al_4

13	-1.210691626	1.281202785	0.199393137
13	1.197852728	1.284810552	-0.200515724
13	-1.197834122	-1.284801757	0.200647570
13	1.210672798	-1.281196192	-0.199523719
3	3.421778765	0.015326589	0.610079677
3	-3.421777823	-0.015393267	-0.610085154

$NaAl_4{}^-$

13	0.000000000	1.813309136	-0.444291034
13	-1.813309136	0.000000000	-0.444291034
13	1.813309136	0.000000000	-0.444291034
13	0.000000000	-1.813309136	-0.444291034
11	0.000000000	0.000000000	2.100286160

Na_2Al_4

13	0.000000000	1.820069984	0.000000000
13	-1.820069984	0.000000000	0.000000000
13	1.820069984	0.000000000	0.000000000
13	0.000000000	-1.820069984	0.000000000
11	0.000000000	0.000000000	2.586693928
11	0.000000000	0.000000000	-2.586693928

$KAl_4{}^-$

13	0.000000000	1.805964140	-0.781585060
13	-1.805964140	0.000000000	-0.781585060
13	1.805964140	0.000000000	-0.781585060
13	0.000000000	-1.805964140	-0.781585060
19	0.000000000	0.000000000	2.139074164

K_2Al_4

13	-0.000000422	1.805590372	0.000000000
13	-1.805590372	-0.000000422	0.000000000
13	1.805590372	0.000000422	0.000000000
13	0.000000422	-1.805590372	0.000000000
19	0.000000000	0.000000000	2.992914277
19	0.000000000	0.000000000	-2.992914277

$BeAl_4$

13	2.134531000	0.212700000	0.000000000
13	0.000000000	1.420864000	0.000000000
13	0.372707000	-1.559301000	0.000000000
13	-1.845769000	-0.594103000	0.000000000
4	-2.149775000	1.689483000	0.000000000

$MgAl_4$

13	0.000000000	1.864442142	-0.396056030
13	-1.864442142	0.000000000	-0.396056030
13	1.864442142	0.000000000	-0.396056030
13	0.000000000	-1.864442142	-0.396056030
12	0.000000000	0.000000000	1.716243132

$CaAl_4$

13	0.000000000	1.831336141	-0.655418049
13	-1.831336141	0.000000000	-0.655418049
13	1.831336141	0.000000000	-0.655418049
13	0.000000000	-1.831336141	-0.655418049
20	0.000000000	0.000000000	1.704087132

T-shaped Benzene-LiAl$_4$$^-$

13	2.238473205	0.982263609	-1.523036418
13	2.231333159	-1.521286471	-0.982018076
13	2.243839845	1.519934651	0.983454427
13	2.231462437	-0.984004555	1.524798033
6	-3.773282044	1.205431985	0.004961232
6	-2.387017910	1.197999955	-0.002614904
6	-1.700918276	-0.005243690	-0.008461149
6	-2.399154918	-1.201657671	-0.007031482
6	-3.785380311	-1.196230757	0.000420010
6	-4.472836449	0.007994748	0.005997129
1	-4.312151698	2.146791209	0.009751809
1	-1.829383445	2.128449153	-0.003391643
1	-0.614216456	-0.010812993	-0.014563495
1	-1.850605236	-2.137497587	-0.010968538

1	-4.333009896	-2.132436356	0.001168445
1	-5.557547159	0.013745530	0.011904864
3	4.440680295	-0.005933462	0.001633333

PPS Benzene-LiAl$_4^-$

13	0.000000000	1.805526881	1.490641377
13	1.811433325	0.000137321	1.497596666
13	-1.811433325	-0.000137321	1.497596666
13	0.000000000	-1.805526881	1.490641377
6	-1.326541369	0.401365720	-2.121975913
6	-0.315269131	1.349333086	-2.120431663
6	1.011813634	0.948665706	-2.117319132
6	1.326541369	-0.401365720	-2.121975913
6	0.315269131	-1.349333086	-2.120431663
6	-1.011813634	-0.948665706	-2.117319132
1	-2.363245659	0.716636236	-2.093452640
1	-0.562618902	2.404521167	-2.092186420
1	1.801781116	1.690205342	-2.083635169
1	2.363245659	-0.716636236	-2.093452640
1	0.562618902	-2.404521167	-2.092186420
1	-1.801781116	-1.690205342	-2.083635169
3	0.000000000	0.000000000	3.720359953

T-shaped Benzene-NaAl$_4^-$

13	0.948961125	1.548790876	1.852653073
13	-1.546659266	0.945266113	1.855124072
13	1.546659266	-0.945266113	1.855124072
13	-0.948961125	-1.548790876	1.852653073
1	0.000000000	0.000000000	-0.976245144
6	0.000000000	0.000000000	-2.063086227
6	-1.199774170	0.004594050	-2.755452278
6	1.199774170	-0.004594050	-2.755452278
1	-2.133360765	0.009046711	-2.203370237
1	2.133360765	-0.009046711	-2.203370237
6	-1.200684112	0.004351940	-4.141711384
6	1.200684112	-0.004351940	-4.141711384
1	-2.139646734	0.007883501	-4.684631430
1	2.139646734	-0.007883501	-4.684631430
6	0.000000000	0.000000000	-4.835377438
1	0.000000000	0.000000000	-5.920043524
11	0.000000000	0.000000000	4.402439264

PPS Benzene-NaAl$_4^-$

13	-0.404999416	-1.768046669	1.172947440

13	-1.766607397	0.404181619	1.172441520
13	1.766607397	-0.404181619	1.172441520
13	0.404999416	1.768046669	1.172947440
6	1.200360769	-0.693079276	-2.435848778
6	0.000000000	-1.385891011	-2.436212815
6	-1.201092568	-0.693595737	-2.433484795
6	-1.200360769	0.693079276	-2.435848778
6	0.000000000	1.385891011	-2.436212815
6	1.201092568	0.693595737	-2.433484795
1	2.137895972	-1.236549513	-2.406769790
1	0.000748321	-2.469644122	-2.407465859
1	-2.139509021	-1.235119543	-2.400354823
1	-2.137895972	1.236549513	-2.406769790
1	-0.000748321	2.469644122	-2.407465859
1	2.139509021	1.235119543	-2.400354823
11	0.000000000	0.000000000	3.737783712

T-shaped Benzene-KAl$_4^-$

13	0.000000000	1.808318137	1.503942115
13	-1.804330136	-0.001390000	1.505837115
13	1.804330136	0.001390000	1.505837115
13	0.000000000	-1.808318137	1.503942115
1	0.000000000	0.000000000	-1.395365109
6	0.000000000	0.000000000	-2.482399188
6	-1.033494079	0.608899045	-3.175152242
6	1.033494079	-0.608899045	-3.175152242
1	-1.837092140	1.083170085	-2.622173199
1	1.837092140	-1.083170085	-2.622173199
6	-1.034566081	0.609297045	-4.561444348
6	1.034566081	-0.609297045	-4.561444348
1	-1.843687138	1.085942085	-5.104396388
1	1.843687138	-1.085942085	-5.104396388
6	0.000000000	0.000000000	-5.255365402
1	0.000000000	0.000000000	-6.340116489
19	0.000000000	0.000000000	4.431585336

PPS Benzene-KAl$_4^-$

13	-1.807137591	0.000244038	0.877900854
13	0.000000000	1.804989025	0.877458854
13	0.000000000	-1.804989025	0.877458854
13	1.807137591	-0.000244038	0.877900854
6	-0.368735728	-1.335624898	-2.821034426
6	-1.341072682	-0.348369207	-2.821594428
6	-0.973104800	0.987835967	-2.820193426

6	0.368735728	1.335624898	-2.821034426
6	1.341072682	0.348369207	-2.821594428
6	0.973104800	-0.987835967	-2.820193426
1	-0.658716575	-2.379613482	-2.787851425
1	-2.389633856	-0.621647258	-2.788837425
1	-1.733127384	1.759860027	-2.783661426
1	0.658716575	2.379613482	-2.787851425
1	2.389633856	0.621647258	-2.788837425
1	1.733127384	-1.759860027	-2.783661426
19	0.000000000	0.000000000	3.822906079

PPS Benzene-MgAl$_4$

13	-0.458772114	1.792625593	0.904462118
13	1.788991235	0.458866811	0.900127855
13	-1.788991235	-0.458866811	0.900127855
13	0.458772114	-1.792625593	0.904462118
6	-1.391566013	-0.000153738	-1.996627470
6	-0.696639427	1.204257217	-1.996100399
6	0.696642438	1.207854818	-1.988403849
6	1.391566013	0.000153738	-1.996627470
6	0.696639427	-1.204257217	-1.996100399
6	-0.696642438	-1.207854818	-1.988403849
1	-2.474207106	0.001984531	-2.050285181
1	-1.241423748	2.139936453	-2.048631751
1	1.237020210	2.145990384	-2.024051446
1	2.474207106	-0.001984531	-2.050285181
1	1.241423748	-2.139936453	-2.048631751
1	-1.237020210	-2.145990384	-2.024051446
12	0.000000000	0.000000000	3.091671436

PPS Benzene-CaAl$_4$

13	0.000000000	1.837521165	0.757874109
13	1.841519734	0.000208109	0.762512072
13	-1.841519734	-0.000208109	0.762512072
13	0.000000000	-1.837521165	0.757874109
6	-1.308256962	0.464965693	-2.449730198
6	-0.251428613	1.364925754	-2.450901151
6	1.057092029	0.901034912	-2.448085150
6	1.308256962	-0.464965693	-2.449730198
6	0.251428613	-1.364925754	-2.450901151
6	-1.057092029	-0.901034912	-2.448085150
1	-2.328725184	0.829915596	-2.466024200
1	-0.448549369	2.430679055	-2.470716124
1	1.881636645	1.604142679	-2.458111122
1	2.328725184	-0.829915596	-2.466024200

1	0.448549369	-2.430679055	-2.470716124
1	-1.881636645	-1.604142679	-2.458111122
20	0.000000000	0.000000000	3.172213234

$Al_4{}^{2-}$

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.8170299789E+02	1.0827279957E+00	4.0101657182E+00	4.0101657177E+00 (Bonded)
Al1	Al3	1.8170299789E+02	1.0827279957E+00	4.0101657182E+00	4.0101657177E+00 (Bonded)
Al2	Al3	1.8184004039E+02	8.0864303352E-01	2.9950205256E+00	2.9950205256E+00
Al1	Al4	1.8184004034E+02	8.0864303332E-01	2.9950205253E+00	2.9950205253E+00
Al2	Al4	1.8170299789E+02	1.0827279957E+00	4.0101657177E+00	4.0101657182E+00 (Bonded)
Al3	Al4	1.8170299789E+02	1.0827279957E+00	4.0101657177E+00	4.0101657182E+00 (Bonded)

$LiAl_4{}^-$

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.8041858842E+02	1.0401528221E+00	3.8663519879E+00	3.8663533465E+00 (Bonded)
Al1	Al3	1.8041861149E+02	1.0401486354E+00	3.8663364253E+00	3.8663373356E+00 (Bonded)
Al2	Al3	1.8055810191E+02	7.6104063989E-01	2.8288651074E+00	2.8288647794E+00
Al1	Al4	1.8055810820E+02	7.6104010717E-01	2.8288621332E+00	2.8288636991E+00
Al2	Al4	1.8041849134E+02	1.0401466713E+00	3.8663304832E+00	3.8663312648E+00 (Bonded)
Al3	Al4	1.8041851053E+02	1.0401502503E+00	3.8663433385E+00	3.8663445684E+00 (Bonded)
Al1	Li5	2.9425308915E+01	9.6153182819E-02	3.5741098964E-01	2.1941656473E+00
Al2	Li5	2.9425298719E+01	9.6152860439E-02	3.5740991691E-01	2.1941582907E+00 (Bonded)
Al3	Li5	2.9425302045E+01	9.6153044985E-02	3.5741056145E-01	2.1941625020E+00
Al4	Li5	2.9425292594E+01	9.6153194566E-02	3.5741123115E-01	2.1941659153E+00

Li_2Al_4

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.8001832483E+02	1.0888135340E+00	4.0514878870E+00	4.0513929562E+00 (Bonded)
Al1	Al3	1.8005036762E+02	1.0246654213E+00	3.8127920099E+00	3.8127033322E+00 (Bonded)
Al2	Al3	1.8019453571E+02	7.4479100473E-01	2.7713110980E+00	2.7713115778E+00
Al1	Al4	1.8018675571E+02	7.4327891618E-01	2.7657495352E+00	2.7657511534E+00
Al2	Al4	1.8005029555E+02	1.0246607950E+00	3.8126854578E+00	3.8127770262E+00 (Bonded)
Al3	Al4	1.8001818566E+02	1.0888180609E+00	4.0514105018E+00	4.0515071020E+00 (Bonded)
Al1	Li5	2.8540689459E+01	2.9451347065E-02	1.0958880668E-01	6.9294004476E-01
Al2	Li5	2.8505467298E+01	1.0123387223E-01	3.7668359556E-01	2.3818606259E+00 (Bonded)
Al3	Li5	2.8541286878E+01	2.9584821233E-02	1.1008290526E-01	6.9608046465E-01
Al4	Li5	2.8505019355E+01	1.0075814077E-01	3.7492243890E-01	2.3706674746E+00
Al1	Li6	2.8505041210E+01	1.0076062790E-01	3.7493147419E-01	2.3707254621E+00
Al2	Li6	2.8541297681E+01	2.9585886800E-02	1.1008685109E-01	6.9610537984E-01
Al3	Li6	2.8505469279E+01	1.0123280082E-01	3.7667967414E-01	2.3818348844E+00 (Bonded)
Al4	Li6	2.8540679628E+01	2.9450376322E-02	1.0958525865E-01	6.9291704976E-01
Li5	Li6	4.5151618591E+00	1.7840167735E-03	4.1974876740E-02	4.1974867346E-02

$NaAl_4{}^-$

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7921647044E+02	9.9704716011E-01	3.7187203207E+00	3.7187208655E+00 (Bonded)
Al1	Al3	1.7921652412E+02	9.9705092495E-01	3.7187343626E+00	3.7187337578E+00 (Bonded)
Al2	Al3	1.7935598557E+02	7.1807535685E-01	2.6782301975E+00	2.6782293696E+00
Al1	Al4	1.7935599833E+02	7.1807604197E-01	2.6782323604E+00	2.6782321221E+00
Al2	Al4	1.7921648503E+02	9.9704998128E-01	3.7187313878E+00	3.7187305120E+00 (Bonded)
Al3	Al4	1.7921654133E+02	9.9704850079E-01	3.7187247163E+00	3.7187249901E+00 (Bonded)
Al1	Na5	1.3897880156E+02	1.7296587895E-01	6.4511665505E-01	8.3368867513E-01
Al2	Na5	1.3897878106E+02	1.7296612960E-01	6.4511768441E-01	8.3368988323E-01
Al3	Na5	1.3897882435E+02	1.7296553797E-01	6.4511527837E-01	8.3368703162E-01
Al4	Na5	1.3897881384E+02	1.7296608758E-01	6.4511737575E-01	8.3368968070E-01 (Bonded)

Na$_2$Al$_4$

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7918637941E+02	9.9326235382E-01	3.7049338979E+00	3.7049340351E+00 (Bonded)
Al1	Al3	1.7918636276E+02	9.9324407008E-01	3.7048656984E+00	3.7048663673E+00 (Bonded)
Al2	Al3	1.7932401708E+02	7.1792212483E-01	2.6778968362E+00	2.6778972206E+00
Al1	Al4	1.7932402246E+02	7.1792221487E-01	2.6778970729E+00	2.6778975748E+00
Al2	Al4	1.7918635433E+02	9.9324517056E-01	3.7048699404E+00	3.7048704975E+00 (Bonded)
Al3	Al4	1.7918632076E+02	9.9326071183E-01	3.7049284421E+00	3.7049284675E+00 (Bonded)
Al1	Na5	1.3654974773E+02	9.5822993890E-02	3.5742606865E-01	4.7016467793E-01 (Bonded)
Al2	Na5	1.3654974252E+02	9.5823280281E-02	3.5742715014E-01	4.7016608313E-01
Al3	Na5	1.3654972280E+02	9.5823510404E-02	3.5742805982E-01	4.7016721226E-01
Al4	Na5	1.3654972179E+02	9.5823666093E-02	3.5742864300E-01	4.7016797616E-01
Al1	Na6	1.3654974711E+02	9.5824231926E-02	3.5743068660E-01	4.7017075247E-01 (Bonded)
Al2	Na6	1.3654974222E+02	9.5823886102E-02	3.5742940989E-01	4.7016905566E-01
Al3	Na6	1.3654972255E+02	9.5824013156E-02	3.5742993511E-01	4.7016967906E-01
Al4	Na6	1.3654972163E+02	9.5823982499E-02	3.5742982321E-01	4.7016952864E-01
Na5	Na6	1.0383457124E+02	1.7936597559E-02	8.8007630240E-02	8.8007630240E-02

KAl$_4^-$

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7942000904E+02	1.0045105432E+00	3.7443991721E+00	3.7443976057E+00 (Bonded)
Al1	Al3	1.7941997998E+02	1.0045094428E+00	3.7443950705E+00	3.7443941203E+00 (Bonded)
Al2	Al3	1.7956044667E+02	7.2372660687E-01	2.6977518478E+00	2.6977522918E+00
Al1	Al4	1.7956042960E+02	7.2372589216E-01	2.6977503121E+00	2.6977487603E+00
Al2	Al4	1.7942011090E+02	1.0045138189E+00	3.7444098162E+00	3.7444092287E+00 (Bonded)
Al3	Al4	1.7942008169E+02	1.0045130180E+00	3.7444074469E+00	3.7444062432E+00 (Bonded)
Al1	K5	2.4592741107E+02	1.8021212903E-01	6.7175616158E-01	4.9128143600E-01
Al2	K5	2.4592751371E+02	1.8021267995E-01	6.7175793414E-01	4.9128293786E-01
Al3	K5	2.4592747352E+02	1.8021207845E-01	6.7175580259E-01	4.9128129812E-01
Al4	K5	2.4592755214E+02	1.8021302075E-01	6.7175909910E-01	4.9128386693E-01 (Bonded)

K$_2$Al$_4$

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7884319241E+02	9.8416280442E-01	3.6745493429E+00	3.6745494761E+00 (Bonded)
Al1	Al3	1.7884321789E+02	9.8416291594E-01	3.6745497593E+00	3.6745493691E+00 (Bonded)
Al2	Al3	1.7898381830E+02	7.0294909937E-01	2.6245873480E+00	2.6245869742E+00
Al1	Al4	1.7898383443E+02	7.0294944896E-01	2.6245885581E+00	2.6245881359E+00
Al2	Al4	1.7884322078E+02	9.8416374855E-01	3.6745530012E+00	3.6745522769E+00 (Bonded)
Al3	Al4	1.7884324618E+02	9.8416403888E-01	3.6745535618E+00	3.6745533609E+00 (Bonded)
Al1	K5	2.4388600037E+02	1.2129774306E-01	4.5288700208E-01	3.3293598300E-01
Al2	K5	2.4388599159E+02	1.2129762481E-01	4.5288657699E-01	3.3293565844E-01
Al3	K5	2.4388602633E+02	1.2129764336E-01	4.5288658173E-01	3.3293570934E-01
Al4	K5	2.4388603955E+02	1.2129787414E-01	4.5288741864E-01	3.3293634279E-01 (Bonded)
Al1	K6	2.4388600055E+02	1.2129738449E-01	4.5288566331E-01	3.3293499882E-01
Al2	K6	2.4388599179E+02	1.2129722058E-01	4.5288506774E-01	3.3293454892E-01
Al3	K6	2.4388602652E+02	1.2129724964E-01	4.5288511174E-01	3.3293462869E-01
Al4	K6	2.4388603981E+02	1.2129736363E-01	4.5288551258E-01	3.3293494157E-01 (Bonded)
K5	K6	3.3182546598E+02	2.1799637195E-02	5.9835273564E-02	5.9835273564E-02

MgAl$_4$

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)	
Al1	Al2	1.7376676479E+02	8.5095928696E-01	3.2237726305E+00	3.2237722640E+00	(Bonded)
Al1	Al3	1.7376672614E+02	8.5096007559E-01	3.2237756182E+00	3.2237759597E+00	(Bonded)
Al2	Al3	1.7389194084E+02	6.0057027628E-01	2.2751990946E+00	2.2751995943E+00	
Al1	Al4	1.7389196224E+02	6.0057067678E-01	2.2752008706E+00	2.2752005708E+00	
Al2	Al4	1.7376678673E+02	8.5096129722E-01	3.2237798796E+00	3.2237798215E+00	(Bonded)
Al3	Al4	1.7376674945E+02	8.5095934568E-01	3.2237731945E+00	3.2237724282E+00	(Bonded)
Al1	Mg5	1.4772197453E+02	3.7788185601E-01	1.4315669429E+00	1.6859325745E+00	
Al2	Mg5	1.4772199102E+02	3.7788251590E-01	1.4315692801E+00	1.6859355186E+00	
Al3	Mg5	1.4772195914E+02	3.7788129478E-01	1.4315649684E+00	1.6859300705E+00	
Al4	Mg5	1.4772199376E+02	3.7788236569E-01	1.4315686852E+00	1.6859348484E+00	

CaAl$_4$

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)	
Al1	Al2	1.7524157282E+02	8.9653089082E-01	3.3819094020E+00	3.3819089644E+00	(Bonded)
Al1	Al3	1.7524160181E+02	8.9653241340E-01	3.3819151455E+00	3.3819141353E+00	(Bonded)
Al2	Al3	1.7538393558E+02	6.1191032576E-01	2.3082584630E+00	2.3082580722E+00	
Al1	Al4	1.7538392521E+02	6.1191014141E-01	2.3082580663E+00	2.3082572156E+00	
Al2	Al4	1.7524163652E+02	8.9653299019E-01	3.3819168836E+00	3.3819160750E+00	(Bonded)
Al3	Al4	1.7524166648E+02	8.9653255462E-01	3.3819146680E+00	3.3819144319E+00	(Bonded)
Al1	Ca5	2.5136623338E+02	4.3029097948E-01	1.6231511083E+00	1.1335144123E+00	
Al2	Ca5	2.5136626588E+02	4.3029108450E-01	1.6231512945E+00	1.1335146889E+00	
Al3	Ca5	2.5136630830E+02	4.3029144998E-01	1.6231523983E+00	1.1335156517E+00	
Al4	Ca5	2.5136632585E+02	4.3029146899E-01	1.6231523567E+00	1.1335157018E+00	(Bonded)

Benzene-Al$_4{}^{2-}$ CH-π

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)	
Al1	Al2	1.8045754508E+02	1.0335477875E+00	3.8420402741E+00	3.8408050845E+00	(Bonded)
Al1	Al3	1.8045666419E+02	1.0353657890E+00	3.8487983895E+00	3.8475604295E+00	(Bonded)
Al2	Al3	1.8065224102E+02	7.6061357823E-01	2.8265441946E+00	2.8265437555E+00	
Al1	Al4	1.8053776034E+02	7.5675402177E-01	2.8131059487E+00	2.8131059427E+00	
Al2	Al4	1.8045663624E+02	1.0353662327E+00	3.8475626758E+00	3.8488000304E+00	(Bonded)
Al3	Al4	1.8045757135E+02	1.0335522484E+00	3.8408210654E+00	3.8420568488E+00	(Bonded)
Al1	H5	1.2563886755E+01	3.2157895817E-02	1.1954157549E-01	1.7191620832E+00	
Al2	H5	1.2567992151E+01	3.2038450315E-02	1.1905926785E-01	1.7127765231E+00	(Bonded)
Al3	H5	1.2567994051E+01	3.2038560905E-02	1.1905966032E-01	1.7127824352E+00	
Al4	H5	1.2563886550E+01	3.2158360352E-02	1.1954330206E-01	1.7191869172E+00	
Al1	C6	8.0852838786E+01	1.4880101215E-02	5.5314276556E-02	1.2375971710E-01	
Al2	C6	8.0879167181E+01	1.4232080648E-02	5.2888360248E-02	1.1837004664E-01	
Al3	C6	8.0879179653E+01	1.4232268708E-02	5.2889050885E-02	1.1837161076E-01	
Al4	C6	8.0852838927E+01	1.4880161236E-02	5.5314499556E-02	1.2376021631E-01	
H5	C6	5.1711835126E+00	9.0283809055E-01	4.8265751633E+01	7.5090206083E+00	(Bonded)
Al1	C7	8.0785390271E+01	5.3537057193E-03	1.9901501641E-02	4.4567260055E-02	
Al2	C7	8.0811224893E+01	5.6467862572E-03	2.0984230850E-02	4.7007027430E-02	
Al3	C7	8.0812070298E+01	3.9810849720E-03	1.4794254520E-02	3.3140792295E-02	
Al4	C7	8.0786007942E+01	4.1187074581E-03	1.5310603041E-02	3.4286439338E-02	
H5	C7	5.5969181798E+00	4.1326303511E-02	2.2093054359E+00	3.4402341336E-01	
C6	C7	3.5415571501E+01	1.3851417767E+00	1.1520402446E+01	1.1530699858E+01	(Bonded)
Al1	C8	8.0786009252E+01	4.1187193548E-03	1.5310647297E-02	3.4286537741E-02	
Al2	C8	8.0812059241E+01	3.9810665401E-03	1.4794188323E-02	3.3140638247E-02	
Al3	C8	8.0811238906E+01	5.6468453947E-03	2.0984447354E-02	4.7007518859E-02	
Al4	C8	8.0785391902E+01	5.3537621010E-03	1.9901711189E-02	4.4567728588E-02	
H5	C8	5.5969182774E+00	4.1326315298E-02	2.2093060661E+00	3.4402350515E-01	
C6	C8	3.5415572167E+01	1.3851417739E+00	1.1520402423E+01	1.1530699622E+01	(Bonded)
C7	C8	3.6035813420E+01	8.0167014351E-02	6.6735535417E-01	6.6735534189E-01	
Al1	H9	1.3370196860E+01	8.9328438494E-03	3.3206346380E-02	4.4917496487E-01	
Al2	H9	1.3373383369E+01	1.1162317394E-02	4.1480699702E-02	5.6128077549E-01	

Al3	H9	1.3375574260E+01	6.7846925957E-03	2.5212842682E-02	3.4115832647E-01
Al4	H9	1.3371505177E+01	6.3162682129E-03	2.3479665961E-02	3.1760429270E-01
H5	H9	9.2685893365E-01	6.2909544522E-03	3.3631461533E-01	3.1633142734E-01
C6	H9	5.9540094724E+00	4.7564680446E-02	3.9560156958E-01	2.3917202661E+00
C7	H9	5.4944561473E+00	9.5599447939E-01	7.9582361841E+00	4.8070781705E+01 (Bonded)
C8	H9	5.9673643059E+00	1.0178382127E-02	8.4730580762E-02	5.1180503221E-01
Al1	H10	1.3371502789E+01	6.3162781162E-03	2.3479702824E-02	3.1760484657E-01
Al2	H10	1.3375569840E+01	6.7846661650E-03	2.5212748379E-02	3.4115705749E-01
Al3	H10	1.3373383083E+01	1.1162336862E-02	4.1480765606E-02	5.6128185323E-01
Al4	H10	1.3370194550E+01	8.9328148534E-03	3.3206238522E-02	4.4917358589E-01
H5	H10	9.2685876727E-01	6.2909598763E-03	3.3631490530E-01	3.1633175575E-01
C6	H10	5.9540084377E+00	4.7564645699E-02	3.9560128059E-01	2.3917189398E+00
C7	H10	5.9673631462E+00	1.0178379357E-02	8.4730559270E-02	5.1180498304E-01
C8	H10	5.4944552464E+00	9.5599439907E-01	7.9582353690E+00	4.8070786127E+01 (Bonded)
H9	H10	9.8790318637E-01	1.7019847932E-03	8.5581811634E-02	8.5581826696E-02
Al1	C11	8.0995498849E+01	2.3676325091E-03	8.8012761137E-03	1.9658741846E-02
Al2	C11	8.1021513572E+01	2.4346919379E-03	9.0476485822E-03	2.0215544472E-02
Al3	C11	8.1021572383E+01	2.3422432580E-03	8.7040952784E-03	1.9447931794E-02
Al4	C11	8.0995511638E+01	2.3423995367E-03	8.7074767591E-03	1.9449229395E-02
H5	C11	5.6277265662E+00	8.7216068451E-03	4.6625736579E-01	7.2416566671E-02
C6	C11	3.6163572480E+01	7.5620816551E-02	6.2894806482E-01	6.2788887423E-01
C7	C11	3.5473405916E+01	1.3912951561E+00	1.1581924051E+01	1.1552093578E+01 (Bonded)
C8	C11	3.6117903308E+01	1.0230170459E-01	8.5161695982E-01	8.4942354571E-01
H9	C11	5.9631241468E+00	4.9503298121E-02	2.4892008154E+00	4.1103192937E-01
H10	C11	5.9851056017E+00	5.5382806237E-03	2.7848437567E-01	4.5985020324E-02
Al1	C12	8.0995511579E+01	2.3424034764E-03	8.7074914226E-03	1.9449262078E-02
Al2	C12	8.1021559918E+01	2.3422308267E-03	8.7040504339E-03	1.9447828547E-02
Al3	C12	8.1021526265E+01	2.4347094051E-03	9.0477120873E-03	2.0215689475E-02
Al4	C12	8.0995499139E+01	2.3676275926E-03	8.8012578184E-03	1.9658700995E-02
H5	C12	5.6277265733E+00	8.7216085931E-03	4.6625745923E-01	7.2416581081E-02
C6	C12	3.6163572530E+01	7.5620819298E-02	6.2894808767E-01	6.2788889615E-01
C7	C12	3.6117902694E+01	1.0230170375E-01	8.5161696855E-01	8.4942353756E-01
C8	C12	3.5473406625E+01	1.3912951727E+00	1.1581923977E+01	1.1552093700E+01 (Bonded)
H9	C12	5.9851066626E+00	5.5382836200E-03	2.7848447733E-01	4.5985045137E-02
H10	C12	5.9631231089E+00	4.9503283362E-02	2.4892005114E+00	4.1103180624E-01
C11	C12	3.6224931209E+01	7.5040247565E-02	6.2306833904E-01	6.2306833815E-01
Al1	H13	1.4060774118E+01	5.7947519241E-03	2.1541016816E-02	2.7710527443E-01
Al2	H13	1.4065262482E+01	5.8636806863E-03	2.1790240245E-02	2.8040145066E-01
Al3	H13	1.4065269167E+01	5.8546803112E-03	2.1756790239E-02	2.7997105236E-01
Al4	H13	1.4060779427E+01	5.7841930029E-03	2.1501765755E-02	2.7660034638E-01
H5	H13	9.7697397466E-01	1.8809558801E-03	1.0055595825E-01	8.9947387250E-02
C6	H13	6.2801373543E+00	1.1211920628E-02	9.3250987011E-02	5.3615450380E-01
C7	H13	6.2541034974E+00	5.2052755165E-02	4.3331643494E-01	2.4891648847E+00
C8	H13	6.2767584357E+00	6.7431098664E-03	5.6133441250E-02	3.2245579009E-01
H9	H13	1.0363458485E+00	6.6902078254E-03	3.3640729823E-01	3.1992601232E-01
H10	H13	1.0393559126E+00	6.6971356319E-04	3.3675571210E-02	3.2025730031E-02
C11	H13	5.8105030302E+00	9.7168750674E-01	8.0680400257E+00	4.6466136384E+01 (Bonded)
C12	H13	6.2908900255E+00	1.0913534009E-02	9.0616405448E-02	5.2188564344E-01
Al1	H14	1.4060779503E+01	5.7842192183E-03	2.1501863252E-02	2.7660159768E-01
Al2	H14	1.4065267112E+01	5.8546573224E-03	2.1756708189E-02	2.7996995067E-01
Al3	H14	1.4065264774E+01	5.8637035661E-03	2.1790321884E-02	2.8040254241E-01
Al4	H14	1.4060774279E+01	5.7947257434E-03	2.1540919448E-02	2.7710402014E-01
H5	H14	9.7697398304E-01	1.8809555916E-03	1.0055594283E-01	8.9947372698E-02
C6	H14	6.2801374064E+00	1.1211922178E-02	9.3250999905E-02	5.3615457342E-01
C7	H14	6.2767583731E+00	6.7431096104E-03	5.6133440152E-02	3.2245577513E-01
C8	H14	6.2541036637E+00	5.2052759723E-02	4.3331646491E-01	2.4891650817E+00
H9	H14	1.0393561041E+00	6.6971396477E-04	3.3675585476E-02	3.2025748965E-02
H10	H14	1.0363456744E+00	6.6902075053E-03	3.3640734135E-01	3.1992599432E-01
C11	H14	6.2908900696E+00	1.0913533941E-02	9.0616405018E-02	5.2188563583E-01
C12	H14	5.8105030864E+00	9.7168751833E-01	8.0680401104E+00	4.6466136547E+01 (Bonded)
H13	H14	1.0922027595E+00	2.0976959538E-03	1.0031190646E-01	1.0031190561E-01
Al1	C15	8.1087438389E+01	2.8642275680E-03	1.0647284822E-02	2.3754994086E-02
Al2	C15	8.1113545117E+01	2.8065713439E-03	1.0429603370E-02	2.3276811668E-02
Al3	C15	8.1113557711E+01	2.8065847968E-03	1.0429651743E-02	2.3276923242E-02
Al4	C15	8.1087438565E+01	2.8642213232E-03	1.0647261585E-02	2.3754942293E-02
H5	C15	5.6362406838E+00	4.5138954577E-03	2.4131298773E-01	3.7436815810E-02

C6	C15	3.6190539392E+01	1.0409350834E-01	8.6575910735E-01	8.6331850957E-01	
C7	C15	3.6173127508E+01	7.4184894834E-02	6.1755682393E-01	6.1526596479E-01	
C8	C15	3.6173128189E+01	7.4184865877E-02	6.1755657150E-01	6.1526572464E-01	
H9	C15	5.9896835554E+00	1.0014898835E-02	5.0358451445E-01	8.3060391311E-02	
H10	C15	5.9896825142E+00	1.0014871236E-02	5.0358321528E-01	8.3060162410E-02	
C11	C15	3.5608986549E+01	1.3894749921E+00	1.1536980534E+01	1.1523864440E+01	(Bonded)
C12	C15	3.5608985826E+01	1.3894765422E+00	1.1536993389E+01	1.1523877296E+01	(Bonded)
H13	C15	6.2768201449E+00	5.3385879009E-02	2.5529149215E+00	4.4276553102E-01	
H14	C15	6.2768198464E+00	5.3386582021E-02	2.5529485181E+00	4.4277136158E-01	
Al1	H16	1.4468059082E+01	1.6992608630E-02	6.3167167989E-02	7.8941154928E-01	
Al2	H16	1.4472667142E+01	1.7087708141E-02	6.3500262984E-02	7.9382950856E-01	
Al3	H16	1.4472669356E+01	1.7087780659E-02	6.3500522604E-02	7.9383287744E-01	
Al4	H16	1.4468059152E+01	1.6992530396E-02	6.3166877033E-02	7.8940791483E-01	
H5	H16	1.0057151063E+00	1.8182825695E-03	9.7205441171E-02	8.4470447799E-02	
C6	H16	6.4662361643E+00	8.0903512665E-03	6.7288492837E-02	3.7584675001E-01	
C7	H16	6.4589604665E+00	1.1085266992E-02	9.2280002433E-02	5.1497907007E-01	
C8	H16	6.4589605637E+00	1.1085310713E-02	9.2280364695E-02	5.1498110119E-01	
H9	H16	1.0690935489E+00	2.2416888937E-03	1.1272004157E-01	1.0414028482E-01	
H10	H16	1.0690933567E+00	2.2416966274E-03	1.1272045029E-01	1.0414064410E-01	
C11	H16	6.4545811124E+00	5.3229990230E-02	4.4197510904E-01	2.4728615818E+00	
C12	H16	6.4545812887E+00	5.3229656184E-02	4.4197233479E-01	2.4728460634E+00	
H13	H16	1.1216153111E+00	7.4643431915E-03	3.5694519724E-01	3.4676481119E-01	(Bonded)
H14	H16	1.1216153661E+00	7.4642520665E-03	3.5694083664E-01	3.4676057788E-01	(Bonded)
C15	H16	6.0014436064E+00	9.7425838311E-01	8.0801897123E+00	4.5260315021E+01	(Bonded)

Benzene-LiAl$_4^-$ CH-π

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)	

Al1	Al2	1.8000929224E+02	1.0221816564E+00	3.8046822419E+00	3.8032207769E+00	(Bonded)
Al1	Al3	1.8002852878E+02	1.0208342227E+00	3.7996669329E+00	3.7978168668E+00	(Bonded)
Al2	Al3	1.8023544683E+02	7.4574964406E-01	2.7747030315E+00	2.7744177395E+00	
Al1	Al4	1.8006600805E+02	7.4061254675E-01	2.7566483777E+00	2.7568733684E+00	
Al2	Al4	1.7999590642E+02	1.0194884505E+00	3.7932001936E+00	3.7949675184E+00	(Bonded)
Al3	Al4	1.8001311484E+02	1.0221942247E+00	3.8028764920E+00	3.8050395553E+00	(Bonded)
Al1	C5	8.0731939536E+01	5.0950248901E-04	1.8964291328E-03	4.2388617623E-03	
Al2	C5	8.0762961018E+01	5.1251495778E-04	1.9069091328E-03	4.2639243262E-03	
Al3	C5	8.0771226131E+01	5.9197288843E-04	2.2023209747E-03	4.9249832832E-03	
Al4	C5	8.0725344853E+01	5.2162389217E-04	1.9417049076E-03	4.3397071035E-03	
Al1	C6	8.0640256672E+01	3.6205161238E-03	1.3475993545E-02	3.0154944650E-02	
Al2	C6	8.0672005041E+01	2.1004885517E-03	7.8152661533E-03	1.7494775289E-02	
Al3	C6	8.0679269778E+01	4.1621549701E-03	1.5484494931E-02	3.4666204612E-02	
Al4	C6	8.0634343727E+01	2.2838724020E-03	8.5015397453E-03	1.9022162453E-02	
C5	C6	3.5383440352E+01	1.3902093963E+00	1.1565999340E+01	1.1578925756E+01	(Bonded)
Al1	C7	8.0773437080E+01	1.3007549172E-02	4.8415651989E-02	1.0815376582E-01	
Al2	C7	8.0804870830E+01	1.2222721857E-02	4.5476955518E-02	1.0162816838E-01	
Al3	C7	8.0813244540E+01	1.2094808110E-02	4.4996401195E-02	1.0056460496E-01	
Al4	C7	8.0766810438E+01	1.3075796259E-02	4.8673648098E-02	1.0872121934E-01	
C5	C7	3.6102704125E+01	7.5048990824E-02	6.2437829916E-01	6.2400924812E-01	
C6	C7	3.5406321068E+01	1.3871230511E+00	1.1553219872E+01	1.1533501019E+01	(Bonded)
Al1	C8	8.0642681158E+01	2.2483202750E-03	8.3685166633E-03	1.8725648402E-02	
Al2	C8	8.0672727021E+01	4.1346416132E-03	1.5383718530E-02	3.4436306064E-02	
Al3	C8	8.0682065369E+01	2.0494446179E-03	7.6245634835E-03	1.7069267115E-02	
Al4	C8	8.0635426447E+01	3.5949273941E-03	1.3381841339E-02	2.9941173045E-02	
C5	C8	3.6027744883E+01	1.0315581356E-01	8.5821608942E-01	8.5915672998E-01	
C6	C8	3.6000471966E+01	7.7145581454E-02	6.4253842801E-01	6.4252457720E-01	
C7	C8	3.5407149333E+01	1.3870229195E+00	1.1532668456E+01	1.1552136858E+01	(Bonded)
Al1	C9	8.0730065464E+01	5.2208113705E-04	1.9432483635E-03	4.3436116942E-03	
Al2	C9	8.0761054727E+01	5.8809691590E-04	2.1881261471E-03	4.8928499039E-03	
Al3	C9	8.0769397444E+01	5.1196126764E-04	1.9046531691E-03	4.2594163844E-03	
Al4	C9	8.0723483140E+01	5.0979078580E-04	1.8976570772E-03	4.2413584051E-03	
C5	C9	3.6080835251E+01	7.4392699622E-02	6.1891821262E-01	6.1893253196E-01	
C6	C9	3.6026170151E+01	1.0308040450E-01	8.5854717556E-01	8.5760855669E-01	
C7	C9	3.6101913401E+01	7.4958192030E-02	6.2325428411E-01	6.2363731683E-01	
C8	C9	3.5383360593E+01	1.3902549646E+00	1.1579055683E+01	1.1566646051E+01	(Bonded)

Al1	C10	8.0786504740E+01	5.0266320955E-04	1.8709725176E-03	4.1791372132E-03	
Al2	C10	8.0817602685E+01	3.9468313681E-04	1.4684934883E-03	3.2813919005E-03	
Al3	C10	8.0825917903E+01	3.8515600119E-04	1.4328986285E-03	3.2021833842E-03	
Al4	C10	8.0779910642E+01	5.0470913905E-04	1.8787410372E-03	4.1961470519E-03	
C5	C10	3.5448487555E+01	1.3895802651E+00	1.1560765214E+01	1.1552957301E+01	(Bonded)
C6	C10	3.6065826735E+01	7.4203043465E-02	6.1803030067E-01	6.1692340794E-01	
C7	C10	3.6112848591E+01	1.0360984819E-01	8.6148398205E-01	8.6141130677E-01	
C8	C10	3.6066582966E+01	7.4247111855E-02	6.1838401182E-01	6.1728979212E-01	
C9	C10	3.5447624999E+01	1.3896329888E+00	1.1561471335E+01	1.1553395645E+01	(Bonded)
Al1	H11	1.3696173560E+01	1.7512073243E-04	6.5182028725E-04	8.5878655788E-03	
Al2	H11	1.3701427536E+01	1.9330346002E-04	7.1922219581E-04	9.4795408146E-03	
Al3	H11	1.3702837818E+01	1.9058048257E-04	7.0901793365E-04	9.3460068578E-03	
Al4	H11	1.3695053755E+01	1.7920426100E-04	6.6707410890E-04	8.7881205339E-03	
C5	H11	5.6426432868E+00	9.6988476964E-01	8.0690625710E+00	4.7562843718E+01	(Bonded)
C6	H11	6.0951428895E+00	5.1204204449E-02	4.2647509312E-01	2.5110380636E+00	
C7	H11	6.1259490293E+00	1.0521228104E-02	8.7480771782E-02	5.1595771345E-01	
C8	H11	6.1176738512E+00	6.4061688539E-03	5.3355238975E-02	3.1415650350E-01	
C9	H11	6.1221728683E+00	1.0542076736E-02	8.7707991237E-02	5.1698012379E-01	
C10	H11	6.1056858565E+00	5.2082125532E-02	4.3301030356E-01	2.5540910371E+00	
Al1	H12	1.3351650210E+01	4.9024362259E-03	1.8247453312E-02	2.4657383088E-01	
Al2	H12	1.3357687607E+01	3.0908132806E-03	1.1499957188E-02	1.5545611121E-01	
Al3	H12	1.3356772572E+01	7.6683300809E-03	2.8528543296E-02	3.8568773511E-01	
Al4	H12	1.3351692610E+01	2.6379590228E-03	9.8196000175E-03	1.3267927047E-01	
C5	H12	5.9497520315E+00	4.9508861234E-02	4.1189439366E-01	2.4901067581E+00	
C6	H12	5.4881095530E+00	9.5945424590E-01	7.9912058642E+00	4.8256886590E+01	(Bonded)
C7	H12	5.9538657961E+00	4.8348207565E-02	4.0200045756E-01	2.4317303084E+00	
C8	H12	5.9629176848E+00	1.0095277773E-02	8.4080824344E-02	5.0775394104E-01	
C9	H12	5.9715300525E+00	5.6763725214E-03	4.7226295521E-02	2.8549987264E-01	
C10	H12	5.9735434292E+00	1.0001647981E-02	8.3153607578E-02	5.0304471984E-01	
H11	H12	1.0102994426E+00	6.5577229383E-03	3.2158866808E-01	3.2982843473E-01	
Al1	H13	1.2915617735E+01	2.9424172864E-02	1.0952028661E-01	1.5284258030E+00	
Al2	H13	1.2920450629E+01	2.9695869305E-02	1.1048911554E-01	1.5425389559E+00	(Bonded)
Al3	H13	1.2922246866E+01	2.8763654595E-02	1.0700963010E-01	1.4941154701E+00	
Al4	H13	1.2914617628E+01	2.9313875993E-02	1.0911865375E-01	1.5226964802E+00	
C5	H13	5.7804754263E+00	8.8787590877E-03	7.3867808707E-02	4.6120326137E-01	
C6	H13	5.7567096732E+00	4.3494003485E-02	3.6225754088E-01	2.2592770070E+00	
C7	H13	5.3303666956E+00	9.1593883961E-01	7.6157493972E+00	4.7578042818E+01	(Bonded)
C8	H13	5.7568247998E+00	4.3512880866E-02	3.6240695649E-01	2.2602575843E+00	
C9	H13	5.7803464863E+00	8.8689649963E-03	7.3788032816E-02	4.6069451157E-01	
C10	H13	5.7864137220E+00	4.8214838922E-03	4.0085771892E-02	2.5044987410E-01	
H11	H13	9.8059553643E-01	1.6368780023E-03	8.0271981835E-02	8.5026912622E-02	
H12	H13	9.5375638109E-01	6.2798643070E-03	3.1585320609E-01	3.2620480754E-01	
Al1	H14	1.3357710772E+01	2.5739323886E-03	9.5804838501E-03	1.2941152613E-01	
Al2	H14	1.3360327879E+01	7.6066524105E-03	2.8301993398E-02	3.8244535930E-01	
Al3	H14	1.3363975352E+01	3.0601592017E-03	1.1384732185E-02	1.5385791571E-01	
Al4	H14	1.3355526757E+01	4.7614844695E-03	1.7724260527E-02	2.3939672019E-01	
C5	H14	5.9738510621E+00	5.6919311302E-03	4.7354644466E-02	2.8617748369E-01	
C6	H14	5.9649749456E+00	1.0099700749E-02	8.4119475415E-02	5.0779021746E-01	
C7	H14	5.9560382307E+00	4.8387060348E-02	4.0232350648E-01	2.4327924665E+00	
C8	H14	5.4903172431E+00	9.5967249553E-01	7.9928513445E+00	4.8250172684E+01	(Bonded)
C9	H14	5.9517775692E+00	4.9562368718E-02	4.1234909496E-01	2.4918843256E+00	
C10	H14	5.9757298589E+00	1.0012880667E-02	8.3246996028E-02	5.0342509921E-01	
H11	H14	1.0137218275E+00	4.5621443111E-04	2.2372612054E-02	2.2937434578E-02	
H12	H14	9.8776627808E-01	1.7063637019E-03	8.5823581474E-02	8.5792125608E-02	
H13	H14	9.5410546280E-01	6.2833970306E-03	3.2638831332E-01	3.1591505767E-01	
Al1	H15	1.3696244426E+01	1.7784440645E-04	6.6195812731E-04	8.7213877022E-03	
Al2	H15	1.3701502912E+01	1.8706206146E-04	6.9599988836E-04	9.1734162179E-03	
Al3	H15	1.3702909044E+01	1.9265371783E-04	7.1673100563E-04	9.4476278398E-03	
Al4	H15	1.3695128758E+01	1.7364266315E-04	6.4637148770E-04	8.5153366205E-03	
C5	H15	6.1223440591E+00	1.0547853187E-02	8.7754019881E-02	5.1726067133E-01	
C6	H15	6.1175762892E+00	6.4019609483E-03	5.3321341889E-02	3.1394849352E-01	
C7	H15	6.1259837559E+00	1.0516441079E-02	8.7440969141E-02	5.1572023957E-01	
C8	H15	6.0952985806E+00	5.1221267366E-02	4.2660801226E-01	2.5118615773E+00	
C9	H15	5.6425289047E+00	9.6989463041E-01	8.0693312971E+00	4.7563076462E+01	(Bonded)
C10	H15	6.1057230773E+00	5.2072355694E-02	4.3292907721E-01	2.5535984608E+00	
H11	H15	1.0385642546E+00	1.9790072611E-03	9.7049892960E-02	9.7049381167E-02	

H12	H15	1.0133553610E+00	4.5657638681E-04	2.2964049627E-02	2.2390244172E-02
H13	H15	9.8060273686E-01	1.6328281778E-03	8.4816546254E-02	8.0072957446E-02
H14	H15	1.0106725252E+00	6.5655132301E-03	3.3009922509E-01	3.2196900362E-01
Al1	H16	1.3752145124E+01	7.7022485791E-05	2.8668689375E-04	3.7617988398E-03
Al2	H16	1.3757428405E+01	7.9573443507E-05	2.9606809294E-04	3.8863882980E-03
Al3	H16	1.3758843854E+01	7.8022513138E-05	2.9026771418E-04	3.8106404433E-03
Al4	H16	1.3751022874E+01	7.6868195300E-05	2.8613595790E-04	3.7542632509E-03
C5	H16	6.1266012544E+00	5.2007307934E-02	4.3268049464E-01	2.5400508519E+00
C6	H16	6.1404629428E+00	1.0546709529E-02	8.7842570289E-02	5.1510411877E-01
C7	H16	6.1529522669E+00	6.5828199615E-03	5.4734120867E-02	3.2150669041E-01
C8	H16	6.1405918147E+00	1.0553931054E-02	8.7900822837E-02	5.1545681998E-01
C9	H16	6.1264765474E+00	5.1972034264E-02	4.3239703521E-01	2.5383280764E+00
C10	H16	5.6711662267E+00	9.7119367647E-01	8.0744951241E+00	4.7433359335E+01 (Bonded)
H11	H16	1.0403422645E+00	6.9010776658E-03	3.3842667581E-01	3.3705048194E-01
H12	H16	1.0167586070E+00	1.9163752589E-03	9.6386361235E-02	9.3596281029E-02
H13	H16	9.8523093094E-01	3.8041301064E-04	1.9760387622E-02	1.8579473349E-02
H14	H16	1.0171286530E+00	1.9225794486E-03	9.6662966615E-02	9.3899295317E-02
H15	H16	1.0403532528E+00	6.8901101276E-03	3.3788704933E-01	3.3651482444E-01
Al1	Li17	2.9318544821E+01	9.1487773804E-02	3.4052842386E-01	2.0926339887E+00
Al2	Li17	2.9329562287E+01	9.2020492822E-02	3.4237970132E-01	2.1048190696E+00
Al3	Li17	2.9332330879E+01	9.2524660182E-02	3.4422015564E-01	2.1163510778E+00 (Bonded)
Al4	Li17	2.9316247927E+01	9.1288672716E-02	3.3981507841E-01	2.0880798752E+00
C5	Li17	1.3137291911E+01	6.0500188023E-05	5.0333794075E-04	1.3838433762E-03
C6	Li17	1.3122515943E+01	2.8009526872E-04	2.3328876426E-03	6.4067235984E-03
C7	Li17	1.3143888927E+01	2.4057976504E-03	2.0003466622E-02	5.5028707378E-02
C8	Li17	1.3122801328E+01	2.7509154438E-04	2.2911626941E-03	6.2922715444E-03
C9	Li17	1.3136987550E+01	6.1343963677E-05	5.1036963239E-04	1.4031433716E-03
C10	Li17	1.3146191121E+01	1.9451709323E-05	1.6172132901E-04	4.4492620573E-04
H11	Li17	2.2287299147E+00	4.8016997350E-05	2.3547384311E-03	1.0983106979E-03
H12	Li17	2.1728611556E+00	4.2817290692E-04	2.1535462997E-02	9.7937586718E-03
H13	Li17	2.1021691932E+00	3.8937818816E-03	2.0226079851E-01	8.9063925935E-02
H14	Li17	2.1736656279E+00	4.1275356029E-04	2.0752319831E-02	9.4410662028E-03
H15	Li17	2.2287417883E+00	4.7776488084E-05	2.3429315769E-03	1.0928094397E-03
H16	Li17	2.2378500567E+00	7.9589541937E-06	3.8871745496E-04	1.8204812914E-04

Benzene-LiAl$_4^-$ π-π

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7965860601E+02	9.9947561338E-01	3.7233349909E+00	3.7230418690E+00 (Bonded)
Al1	Al3	1.7965837792E+02	9.9940819018E-01	3.7230838200E+00	3.7227961279E+00 (Bonded)
Al2	Al3	1.7981433052E+02	7.1587131722E-01	2.6666172252E+00	2.6666211004E+00
Al1	Al4	1.7978624066E+02	7.1579622577E-01	2.6665474355E+00	2.6665477607E+00
Al2	Al4	1.7965861224E+02	9.9941922039E-01	3.7228318054E+00	3.7231253647E+00 (Bonded)
Al3	Al4	1.7965832790E+02	9.9946427701E-01	3.7230050514E+00	3.7232932137E+00 (Bonded)
Al1	C5	8.0660889381E+01	1.8508970903E-02	6.8951256124E-02	1.5397476156E-01
Al2	C5	8.0668530383E+01	1.5929578302E-02	5.9337602821E-02	1.3251698507E-01
Al3	C5	8.0656184699E+01	4.0386466634E-02	1.5043961325E-01	3.3597203230E-01 (Bonded)
Al4	C5	8.0663738673E+01	1.2790709607E-02	4.7649088990E-02	1.0640496828E-01
Al1	C6	8.0654882732E+01	4.1919387812E-02	1.5616181260E-01	3.4869965811E-01 (Bonded)
Al2	C6	8.0675801139E+01	1.2786084930E-02	4.7628105078E-02	1.0635898271E-01
Al3	C6	8.0673500027E+01	1.7153811673E-02	6.3897959115E-02	1.4269121229E-01
Al4	C6	8.0667827269E+01	1.6010637539E-02	5.9644250892E-02	1.3318190287E-01
C5	C6	3.5439372090E+01	1.3759632528E+00	1.1446536648E+01	1.1445728119E+01 (Bonded)
Al1	C7	8.0635713157E+01	2.9743093924E-02	1.1080160522E-01	2.4749060723E-01
Al2	C7	8.0641401813E+01	3.1065314900E-02	1.1571814909E-01	2.5849273340E-01
Al3	C7	8.0649452536E+01	1.4729445896E-02	5.4867195093E-02	1.2256288866E-01
Al4	C7	8.0643364840E+01	1.4420056761E-02	5.3718877919E-02	1.1998847912E-01
C5	C7	3.6079996793E+01	7.2092583937E-02	5.9973287980E-01	5.9987832540E-01
C6	C7	3.5431683401E+01	1.3738218628E+00	1.1427915313E+01	1.1431494246E+01 (Bonded)
Al1	C8	8.0663743107E+01	1.2790378929E-02	4.7647851308E-02	1.0640222474E-01
Al2	C8	8.0656297181E+01	4.0384841378E-02	1.5043334055E-01	3.3595853511E-01 (Bonded)
Al3	C8	8.0668407529E+01	1.5929666502E-02	5.9338017595E-02	1.3251772795E-01
Al4	C8	8.0660874019E+01	1.8508879135E-02	6.8950922672E-02	1.5397400878E-01
C5	C8	3.6076978562E+01	9.5641588506E-02	7.9563530909E-01	7.9563536402E-01

C6	C8	3.6091198434E+01	7.2305575053E-02	6.0146224971E-01	6.0150477869E-01	
C7	C8	3.5429191344E+01	1.3736984954E+00	1.1430467713E+01	1.1427697088E+01	(Bonded)
Al1	C9	8.0667867871E+01	1.6010532672E-02	5.9643852958E-02	1.3318097985E-01	
Al2	C9	8.0673648729E+01	1.7152333782E-02	6.3892361122E-02	1.4267886438E-01	
Al3	C9	8.0675714125E+01	1.2787044061E-02	4.7631747052E-02	1.0636692059E-01	
Al4	C9	8.0654903632E+01	4.1919334471E-02	1.5616163293E-01	3.4869908165E-01	(Bonded)
C5	C9	3.6091214478E+01	7.2305982155E-02	6.0150812382E-01	6.0146540716E-01	
C6	C9	3.6081957982E+01	9.5923066757E-02	7.9792054055E-01	7.9792023680E-01	
C7	C9	3.6082538024E+01	7.2140116318E-02	6.0027383966E-01	6.0008567950E-01	
C8	C9	3.5439383213E+01	1.3759635235E+00	1.1446539690E+01	1.1445726014E+01	(Bonded)
Al1	C10	8.0643385748E+01	1.4419999894E-02	5.3718659520E-02	1.1998798950E-01	
Al2	C10	8.0649580898E+01	1.4729235001E-02	5.4866329777E-02	1.2256111703E-01	
Al3	C10	8.0641294651E+01	3.1067304817E-02	1.1572572970E-01	2.5850925599E-01	
Al4	C10	8.0635714035E+01	2.9743753897E-02	1.1080407732E-01	2.4749606493E-01	
C5	C10	3.5429198780E+01	1.3736985010E+00	1.1427696346E+01	1.1430466195E+01	(Bonded)
C6	C10	3.6082529254E+01	7.2140047788E-02	6.0008533788E-01	6.0027318723E-01	
C7	C10	3.6060217199E+01	9.4148379109E-02	7.8340335322E-01	7.8340324595E-01	
C8	C10	3.6079999235E+01	7.2092603776E-02	5.9973308626E-01	5.9987840834E-01	
C9	C10	3.5431701655E+01	1.3738227441E+00	1.1427918293E+01	1.1431500014E+01	(Bonded)
Al1	H11	1.3533359620E+01	3.1446157626E-03	1.1714600882E-02	1.5591633231E-01	
Al2	H11	1.3534013375E+01	3.9683643551E-03	1.4782138201E-02	1.9675943334E-01	
Al3	H11	1.3529782051E+01	1.2391671582E-02	4.6158984324E-02	6.1440383503E-01	
Al4	H11	1.3533893087E+01	2.0743815390E-03	7.7276705974E-03	1.0285198122E-01	
C5	H11	5.5797539450E+00	9.6261587290E-01	8.0079303317E+00	4.7728418241E+01	(Bonded)
C6	H11	6.0367220754E+00	4.9535922151E-02	4.1205656903E-01	2.4560899908E+00	
C7	H11	6.0545128022E+00	1.0159046588E-02	8.4532853754E-02	5.0370582713E-01	
C8	H11	6.0582551108E+00	5.6127042779E-03	4.6691675463E-02	2.7828909203E-01	
C9	H11	6.0564194113E+00	1.0145865277E-02	8.4396709763E-02	5.0305227144E-01	
C10	H11	6.0349185710E+00	4.9349168583E-02	4.1063159259E-01	2.4468303757E+00	
Al1	H12	1.3531061557E+01	1.3028138885E-02	4.8533575733E-02	6.4583500838E-01	
Al2	H12	1.3537624352E+01	2.0342244997E-03	7.5774765107E-03	1.0084121826E-01	
Al3	H12	1.3537201199E+01	2.8411812417E-03	1.0583401887E-02	1.4084393230E-01	
Al4	H12	1.3535535934E+01	4.0760840668E-03	1.5184590879E-02	2.0206092449E-01	
C5	H12	6.0374915681E+00	4.9508369757E-02	4.1185647049E-01	2.4542445149E+00	
C6	H12	5.5814345715E+00	9.6247884033E-01	8.0062248060E+00	4.7712304529E+01	(Bonded)
C7	H12	6.0360900556E+00	4.9371708907E-02	4.1081920558E-01	2.4474699202E+00	
C8	H12	6.0571718748E+00	1.0146919217E-02	8.4411477176E-02	5.0300627862E-01	
C9	H12	6.0598591290E+00	5.6343411158E-03	4.6868338861E-02	2.7930733422E-01	
C10	H12	6.0556964571E+00	1.0160565630E-02	8.4545482043E-02	5.0368276290E-01	
H11	H12	1.0138074599E+00	6.6465718716E-03	3.2955031295E-01	3.2948595639E-01	
Al1	H13	1.3518851701E+01	6.9863931523E-03	2.6026329943E-02	3.4672177055E-01	
Al2	H13	1.3519588154E+01	7.6427632433E-03	2.8469256447E-02	3.7929620419E-01	
Al3	H13	1.3521810668E+01	3.1584315107E-03	1.1765159335E-02	1.5674711424E-01	
Al4	H13	1.3520838058E+01	3.0103800573E-03	1.1214535522E-02	1.4939959443E-01	
C5	H13	6.0503488451E+00	1.0152906085E-02	8.4461275659E-02	5.0386995083E-01	
C6	H13	6.0311740526E+00	4.9358004861E-02	4.1057659279E-01	2.4495464917E+00	
C7	H13	5.5724980600E+00	9.6291809764E-01	8.0123871883E+00	4.7787844233E+01	(Bonded)
C8	H13	6.0307716964E+00	4.9306367327E-02	4.1017605552E-01	2.4469838165E+00	
C9	H13	6.0507786543E+00	1.0153412136E-02	8.4459487062E-02	5.0389506518E-01	
C10	H13	6.0512229358E+00	5.4700039994E-03	4.5515588575E-02	2.7146618151E-01	
H11	H13	1.0150538901E+00	1.8650236016E-03	9.2471596399E-02	9.2557671915E-02	
H12	H13	1.0128696417E+00	6.6304137235E-03	3.2868495958E-01	3.2905516990E-01	
Al1	H14	1.3533948649E+01	2.0744750605E-03	7.7280180499E-03	1.0285620816E-01	
Al2	H14	1.3529855496E+01	1.2392047779E-02	4.6160318578E-02	6.1442003820E-01	
Al3	H14	1.3534047601E+01	3.9684968068E-03	1.4782653065E-02	1.9676521613E-01	
Al4	H14	1.3533411856E+01	3.1447583457E-03	1.1715133474E-02	1.5592278026E-01	
C5	H14	6.0582796529E+00	5.6127829982E-03	4.6692327108E-02	2.7829188570E-01	
C6	H14	6.0564412416E+00	1.0145918960E-02	8.4397188438E-02	5.0305292764E-01	
C7	H14	6.0349418364E+00	4.9349292544E-02	4.1063268029E-01	2.4468267675E+00	
C8	H14	5.5797761976E+00	9.6261885661E-01	8.0079557058E+00	4.7728375906E+01	(Bonded)
C9	H14	6.0367478957E+00	4.9537225819E-02	4.1206725652E-01	2.4561448376E+00	
C10	H14	6.0545377428E+00	1.0159139165E-02	8.4533612513E-02	5.0370840924E-01	
H11	H14	1.0167298624E+00	4.1261234487E-04	2.0458144440E-02	2.0458062882E-02	
H12	H14	1.0161965577E+00	1.8764859558E-03	9.3021753431E-02	9.3039551912E-02	
H13	H14	1.0126826314E+00	6.6156415696E-03	3.2832205522E-01	3.2801541911E-01	
Al1	H15	1.3535549074E+01	4.0760505893E-03	1.5184464314E-02	2.0205909369E-01	

Al2	H15	1.3537232369E+01	2.8411383809E-03	1.0583226850E-02	1.4084168823E-01
Al3	H15	1.3537616164E+01	2.0341997632E-03	7.5773953790E-03	1.0083990656E-01
Al4	H15	1.3531071382E+01	1.3028132899E-02	4.8533559354E-02	6.4583416433E-01
C5	H15	6.0571774051E+00	1.0146971101E-02	8.4411902968E-02	5.0300842435E-01
C6	H15	6.0598619441E+00	5.6343711333E-03	4.6868606398E-02	2.7930858555E-01
C7	H15	6.0557007789E+00	1.0160535207E-02	8.4545240473E-02	5.0368082791E-01
C8	H15	6.0374965176E+00	4.9507909044E-02	4.1185266629E-01	2.4542195964E+00
C9	H15	5.5814410644E+00	9.6248074635E-01	8.0062376131E+00	4.7712358579E+01 (Bonded)
C10	H15	6.0360957545E+00	4.9372243641E-02	4.1082359882E-01	2.4474943539E+00
H11	H15	1.0161933764E+00	1.8764628663E-03	9.3038777997E-02	9.3020529995E-02
H12	H15	1.0171234033E+00	4.1374975610E-04	2.0510533359E-02	2.0510515976E-02
H13	H15	1.0152516521E+00	1.8681152058E-03	9.2711102512E-02	9.2606717487E-02
H14	H15	1.0138123250E+00	6.6466755068E-03	3.2955413759E-01	3.2949081459E-01
Al1	H16	1.3520869919E+01	3.0104082145E-03	1.1214639048E-02	1.4940065787E-01
Al2	H16	1.3521860513E+01	3.1585034543E-03	1.1765410227E-02	1.5675033429E-01
Al3	H16	1.3519598820E+01	7.6425840793E-03	2.8468630433E-02	3.7928646481E-01
Al4	H16	1.3518880231E+01	6.9864858790E-03	2.6026678551E-02	3.4672559739E-01
C5	H16	6.0307857164E+00	4.9306234372E-02	4.1017492115E-01	2.4469717485E+00
C6	H16	6.0507898752E+00	1.0153432300E-02	8.4459686944E-02	5.0389493955E-01
C7	H16	6.0512356093E+00	5.4700632919E-03	4.5516088177E-02	2.7146851729E-01
C8	H16	6.0503619204E+00	1.0152990032E-02	8.4461979835E-02	5.0387299065E-01
C9	H16	6.0311894745E+00	4.9358844356E-02	4.1058341970E-01	2.4495826789E+00
C10	H16	5.5725114800E+00	9.6291997978E-01	8.0124017523E+00	4.7787830822E+01 (Bonded)
H11	H16	1.0126808440E+00	6.6156576603E-03	3.2801752458E-01	3.2832211989E-01
H12	H16	1.0152530611E+00	1.8681177444E-03	9.2606921817E-02	9.2711021268E-02
H13	H16	1.0148412281E+00	4.0521916563E-04	2.0110277722E-02	2.0110232771E-02
H14	H16	1.0150602116E+00	1.8650231605E-03	9.2471205886E-02	9.2557443137E-02
H15	H16	1.0128725188E+00	6.6309248188E-03	3.2871001718E-01	3.2907979903E-01
Al1	Li17	2.9450152229E+01	9.5662357170E-02	3.5636987736E-01	2.1763505519E+00
Al2	Li17	2.9452431799E+01	9.5748077104E-02	3.5666112826E-01	2.1783007090E+00
Al3	Li17	2.9452389434E+01	9.5747067068E-02	3.5665788418E-01	2.1782777304E+00
Al4	Li17	2.9450148608E+01	9.5662404879E-02	3.5637009854E-01	2.1763516373E+00 (Bonded)
C5	Li17	1.3208595748E+01	1.7227276797E-03	1.4331244298E-02	3.9192629655E-02
C6	Li17	1.3209529248E+01	1.7219671918E-03	1.4323906011E-02	3.9175328302E-02
C7	Li17	1.3205399102E+01	1.7105286721E-03	1.4233212618E-02	3.8915098161E-02
C8	Li17	1.3208594868E+01	1.7226638565E-03	1.4330714347E-02	3.9191177657E-02
C9	Li17	1.3209534269E+01	1.7219816806E-03	1.4324021080E-02	3.9175657926E-02
C10	Li17	1.3205400921E+01	1.7105075998E-03	1.4233035328E-02	3.8914618759E-02
H11	Li17	2.2161988487E+00	1.9890516224E-04	9.8621153476E-03	4.5251588236E-03
H12	Li17	2.2166314503E+00	1.9949491781E-04	9.8894249637E-03	4.5385759596E-03
H13	Li17	2.2141429081E+00	1.8862093238E-04	9.3609080126E-03	4.2911891620E-03
H14	Li17	2.2162076807E+00	1.9891207905E-04	9.8624189790E-03	4.5253161831E-03
H15	Li17	2.2166333290E+00	1.9949489835E-04	9.8894156180E-03	4.5385755169E-03
H16	Li17	2.2141478562E+00	1.8862333701E-04	9.3610064257E-03	4.2912438681E-03

Benzene-NaAl$_4^-$ CH-π

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7882322313E+02	9.7845070927E-01	3.6541838008E+00	3.6527259048E+00 (Bonded)
Al1	Al3	1.7882207642E+02	9.8081370214E-01	3.6630087832E+00	3.6615466560E+00 (Bonded)
Al2	Al3	1.7903203266E+02	7.0403759045E-01	2.6282942209E+00	2.6282937110E+00
Al1	Al4	1.7889087699E+02	7.0004761189E-01	2.6144420142E+00	2.6144421320E+00
Al2	Al4	1.7882203432E+02	9.8081217279E-01	3.6615416570E+00	3.6630032365E+00 (Bonded)
Al3	Al4	1.7882324917E+02	9.7845205350E-01	3.6527302144E+00	3.6541889856E+00 (Bonded)
Al1	H5	1.2895886231E+01	2.8404099616E-02	1.0607974394E-01	1.4727885126E+00
Al2	H5	1.2901153291E+01	2.8175469730E-02	1.0518390675E-01	1.4609337636E+00 (Bonded)
Al3	H5	1.2901155853E+01	2.8175356472E-02	1.0518346353E-01	1.4609278911E+00
Al4	H5	1.2895885729E+01	2.8403939551E-02	1.0607915093E-01	1.4727802130E+00
Al1	C6	8.0497772134E+01	1.2731388826E-02	4.7547448602E-02	1.0586347648E-01
Al2	C6	8.0530448966E+01	1.1640231015E-02	4.3454997748E-02	9.6790329730E-02
Al3	C6	8.0530464581E+01	1.1640249823E-02	4.3455059528E-02	9.6790486114E-02
Al4	C6	8.0497768549E+01	1.2731307954E-02	4.7547148715E-02	1.0586280402E-01
H5	C6	5.3402984532E+00	9.1625933458E-01	4.7509206091E+01	7.6188387494E+00 (Bonded)
Al1	C7	8.0367608824E+01	3.6654569790E-03	1.3689247080E-02	3.0529925815E-02

Al2	C7	8.0399376185E+01	4.2857189762E-03	1.5999330959E-02	3.5696144617E-02
Al3	C7	8.0400501491E+01	2.0663027680E-03	7.7138644923E-03	1.7210424398E-02
Al4	C7	8.0368284173E+01	2.3075177557E-03	8.6178019013E-03	1.9219526052E-02
H5	C7	5.7669393080E+00	4.3574232658E-02	2.2593791097E+00	3.6293376191E-01
C6	C7	3.5403587576E+01	1.3869756223E+00	1.1532917829E+01	1.1552246582E+01 (Bonded)
Al1	C8	8.0368288301E+01	2.3074988683E-03	8.6177309753E-03	1.9219368618E-02
Al2	C8	8.0400486415E+01	2.0662540620E-03	7.7136841609E-03	1.7210018614E-02
Al3	C8	8.0399392388E+01	4.2855053696E-03	1.5998530425E-02	3.5694365247E-02
Al4	C8	8.0367605639E+01	3.6655821291E-03	1.3689715091E-02	3.0530968013E-02
H5	C8	5.7669393969E+00	4.3574126646E-02	2.2593736128E+00	3.6293287668E-01
C6	C8	3.5403587814E+01	1.3869755936E+00	1.1532917590E+01	1.1552246271E+01 (Bonded)
C7	C8	3.5998119305E+01	7.7120270403E-02	6.4234177288E-01	6.4234176890E-01
Al1	H9	1.3307163975E+01	4.7907442849E-03	1.7891816107E-02	2.4095053011E-01
Al2	H9	1.3310831108E+01	8.0808472609E-03	3.0167201927E-02	4.0642629108E-01
Al3	H9	1.3313339485E+01	3.0692604904E-03	1.1458078594E-02	1.5436848602E-01
Al4	H9	1.3308287969E+01	2.5415583021E-03	9.4918645432E-03	1.2782769937E-01
H5	H9	9.5550366017E-01	6.2735865329E-03	3.2529340142E-01	3.1553009530E-01
C6	H9	5.9536963220E+00	4.8299914306E-02	4.0162129303E-01	2.4292446568E+00
C7	H9	5.4881615074E+00	9.5936576090E-01	7.9906450078E+00	4.8251310216E+01 (Bonded)
C8	H9	5.9628021263E+00	1.0084597033E-02	8.3995528838E-02	5.0720490522E-01
Al1	H10	1.3308294067E+01	2.5415656908E-03	9.4918917102E-03	1.2782801814E-01
Al2	H10	1.3313342397E+01	3.0692779604E-03	1.1458146035E-02	1.5436930086E-01
Al3	H10	1.3310839134E+01	8.0809709547E-03	3.0167657845E-02	4.0643234423E-01
Al4	H10	1.3307168908E+01	4.7906842609E-03	1.7891592743E-02	2.4094741159E-01
H5	H10	9.5550408793E-01	6.2735236624E-03	3.2529014150E-01	3.1552680278E-01
C6	H10	5.9536987877E+00	4.8299925664E-02	4.0162138747E-01	2.4292442237E+00
C7	H10	5.9628045541E+00	1.0084601929E-02	8.3995570138E-02	5.0720494178E-01
C8	H10	5.4881637231E+00	9.5936633798E-01	7.9906497648E+00	4.8251319292E+01 (Bonded)
H9	H10	9.8744946390E-01	1.7083587640E-03	8.5921920545E-02	8.5921885023E-02
Al1	C11	8.0460218620E+01	5.3162520838E-04	1.9854410714E-03	4.4229445629E-03
Al2	C11	8.0492288955E+01	6.1861335149E-04	2.3093907467E-03	5.1466569237E-03
Al3	C11	8.0492344357E+01	5.3904326359E-04	2.0123414415E-03	4.4846603101E-03
Al4	C11	8.0460205158E+01	5.5130126581E-04	2.0589246106E-03	4.5866428035E-03
H5	C11	5.7908378232E+00	8.8921951889E-03	4.6107157427E-01	7.3980100536E-02
C6	C11	3.6100445669E+01	7.5041309686E-02	6.2398015111E-01	6.2431868813E-01
C7	C11	3.5382425816E+01	1.3901518403E+00	1.1578701591E+01	1.1565600025E+01 (Bonded)
C8	C11	3.6025931014E+01	1.0314189138E-01	8.5907822432E-01	8.5810616296E-01
H9	C11	5.9498554857E+00	4.9498608377E-02	2.4895329867E+00	4.1181192566E-01
H10	C11	5.9717711074E+00	5.6723051445E-03	2.8528852412E-01	4.7191688435E-02
Al1	C12	8.0460213299E+01	5.5130148114E-04	2.0589253221E-03	4.5866443374E-03
Al2	C12	8.0492333260E+01	5.3904224499E-04	2.0123380293E-03	4.4846515839E-03
Al3	C12	8.0492309090E+01	6.1861503991E-04	2.3093966018E-03	5.1466706819E-03
Al4	C12	8.0460219514E+01	5.3162406617E-04	1.9854368951E-03	4.4229348118E-03
H5	C12	5.7908381479E+00	8.8921965477E-03	4.6107164472E-01	7.3980107687E-02
C6	C12	3.6100447691E+01	7.5041321999E-02	6.2398025349E-01	6.2431875552E-01
C7	C12	3.6025932810E+01	1.0314190234E-01	8.5907832092E-01	8.5810620596E-01
C8	C12	3.5382428068E+01	1.3901518340E+00	1.1578701467E+01	1.1565599324E+01 (Bonded)
H9	C12	5.9717689662E+00	5.6723183966E-03	2.8528930858E-01	4.7191796039E-02
H10	C12	5.9498582877E+00	4.9498615423E-02	2.4895323119E+00	4.1181196117E-01
C11	C12	3.6081167709E+01	7.4409635339E-02	6.1906336807E-01	6.1906333332E-01
Al1	H13	1.3651744203E+01	1.8355180612E-04	6.8550416509E-04	9.0002831689E-03
Al2	H13	1.3657183951E+01	2.0164786767E-04	7.5278640296E-04	9.8876058362E-03
Al3	H13	1.3657184509E+01	2.0582983300E-04	7.6839825451E-04	1.0092664413E-02
Al4	H13	1.3651741385E+01	1.8795728832E-04	7.0195718871E-04	9.2163016769E-03
H5	H13	9.8247472960E-01	1.6373963617E-03	8.4901073601E-02	8.0288128058E-02
C6	H13	6.1263184852E+00	1.0515366840E-02	8.7436909314E-02	5.1561072149E-01
C7	H13	6.0957034343E+00	5.1227256731E-02	4.2667649811E-01	2.5118783971E+00
C8	H13	6.1181135701E+00	6.4070609566E-03	5.3364995309E-02	3.1416396334E-01
H9	H13	1.0104326331E+00	6.5728036399E-03	3.3057922259E-01	3.2229099360E-01
H10	H13	1.0134921376E+00	4.5463290868E-04	2.2865757082E-02	2.2292479722E-02
C11	H13	5.6433087428E+00	9.6988515307E-01	8.0691212471E+00	4.7557369243E+01 (Bonded)
C12	H13	6.1229793831E+00	1.0544560660E-02	8.7727225656E-02	5.1704221186E-01
Al1	H14	1.3651741321E+01	1.8795633942E-04	7.0195361326E-04	9.2162556075E-03
Al2	H14	1.3657181180E+01	2.0582906295E-04	7.6839552886E-04	1.0092627157E-02
Al3	H14	1.3657185920E+01	2.0164732211E-04	7.5278422022E-04	9.8875795774E-03
Al4	H14	1.3651742909E+01	1.8355054297E-04	6.8549947850E-04	9.0002216796E-03

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H5	H14	9.8247468008E-01	1.6373974188E-03	8.4901128410E-02	8.0288183890E-02
C6	H14	6.1263181775E+00	1.0515371222E-02	8.7436945747E-02	5.1561096202E-01
C7	H14	6.1181132327E+00	6.4070500578E-03	5.3364904863E-02	3.1416344458E-01
C8	H14	6.0957031728E+00	5.1227245683E-02	4.2667640344E-01	2.5118779805E+00
H9	H14	1.0134916679E+00	4.5463307391E-04	2.2865774846E-02	2.2292488935E-02
H10	H14	1.0104329966E+00	6.5728139793E-03	3.3057960594E-01	3.2229151664E-01
C11	H14	6.1229787364E+00	1.0544555342E-02	8.7727186343E-02	5.1704197689E-01
C12	H14	5.6433087151E+00	9.6988528591E-01	8.0691218993E+00	4.7557378125E+01 (Bonded)
H13	H14	1.0387974749E+00	1.9818330828E-03	9.7177245572E-02	9.7177250414E-02
Al1	C15	8.0513805629E+01	5.3063548043E-04	1.9817447709E-03	4.4117721252E-03
Al2	C15	8.0546007850E+01	3.9662938977E-04	1.4806861837E-03	3.2976281277E-03
Al3	C15	8.0546023475E+01	3.9663073666E-04	1.4806909246E-03	3.2976393259E-03
Al4	C15	8.0513802003E+01	5.3063463695E-04	1.9817417101E-03	4.4117651124E-03
H5	C15	5.7967256602E+00	4.8358152508E-03	2.5074314083E-01	4.0205594448E-02
C6	C15	3.6110217266E+01	1.0363373417E-01	8.6173060383E-01	8.6162429109E-01
C7	C15	3.6064406014E+01	7.4246524760E-02	6.1840608306E-01	6.1729522509E-01
C8	C15	3.6064406239E+01	7.4246521720E-02	6.1840605391E-01	6.1729519981E-01
H9	C15	5.9735860514E+00	9.9956255859E-03	5.0273008544E-01	8.3104926000E-02
H10	C15	5.9735885204E+00	9.9956310468E-03	5.0273015226E-01	8.3104971402E-02
C11	C15	3.5447628826E+01	1.3895928637E+00	1.1560949527E+01	1.1553255083E+01 (Bonded)
C12	C15	3.5447630819E+01	1.3895929370E+00	1.1560949487E+01	1.1553255692E+01 (Bonded)
H13	C15	6.1062961082E+00	5.2073227323E-02	2.5533597371E+00	4.3294355777E-01
H14	C15	6.1062958070E+00	5.2073218725E-02	2.5533594427E+00	4.3294348628E-01
Al1	H16	1.3709785704E+01	8.5622905908E-05	3.1977271086E-04	4.1806760209E-03
Al2	H16	1.3715256346E+01	8.8223351294E-05	3.2935304521E-04	4.3076469471E-03
Al3	H16	1.3715259007E+01	8.8223315565E-05	3.2935284793E-04	4.3076452026E-03
Al4	H16	1.3709785087E+01	8.5622772461E-05	3.1977222688E-04	4.1806695051E-03
H5	H16	9.8727929402E-01	3.8226188157E-04	1.9820762340E-02	1.8664550859E-02
C6	H16	6.1543289896E+00	6.5878137049E-03	5.4778694671E-02	3.2166059414E-01
C7	H16	6.1420414695E+00	1.0557481403E-02	8.7934226448E-02	5.1548600078E-01
C8	H16	6.1420415062E+00	1.0557484262E-02	8.7934249719E-02	5.1548614039E-01
H9	H16	1.0170673786E+00	1.9158010317E-03	9.6355231406E-02	9.3542065049E-02
H10	H16	1.0170677987E+00	1.9158024718E-03	9.6355263999E-02	9.3542135364E-02
C11	H16	6.1282787023E+00	5.2010442135E-02	4.3270954543E-01	2.5394934447E+00
C12	H16	6.1282790378E+00	5.2010462155E-02	4.3270968769E-01	2.5394944222E+00
H13	H16	1.0407586956E+00	6.8934674924E-03	3.3801443177E-01	3.3658463165E-01
H14	H16	1.0407586418E+00	6.8934709553E-03	3.3801461841E-01	3.3658480074E-01
C15	H16	5.6727780773E+00	9.7120917270E-01	8.0747588766E+00	4.7420849088E+01 (Bonded)
Al1	Na17	1.3868870084E+02	1.6452812662E-01	6.1445713040E-01	7.9365200487E-01
Al2	Na17	1.3874327811E+02	1.6614764075E-01	6.2025790942E-01	8.0146422924E-01 (Bonded)
Al3	Na17	1.3874330497E+02	1.6614778639E-01	6.2025833279E-01	8.0146493180E-01
Al4	Na17	1.3868869471E+02	1.6452788882E-01	6.1445626998E-01	7.9365085777E-01
H5	Na17	9.9909576931E+00	8.4475170594E-03	4.3801445048E-01	4.0749195826E-02
C6	Na17	6.2324835057E+01	5.3202647500E-03	4.4238828140E-02	2.5663932801E-02
C7	Na17	6.2222899884E+01	6.2290853823E-04	5.1882620833E-03	3.0047908548E-03
C8	Na17	6.2222900274E+01	6.2290037292E-04	5.1881940416E-03	3.0047514670E-03
H9	Na17	1.0303971056E+01	9.7361687951E-04	4.8968070364E-02	4.6965403684E-03
H10	Na17	1.0303975314E+01	9.7362202243E-04	4.8968308783E-02	4.6965651769E-03
C11	Na17	6.2293632370E+01	1.3142726078E-04	1.0934310099E-03	6.3397980124E-04
C12	Na17	6.2293635868E+01	1.3142723442E-04	1.0934307292E-03	6.3397967409E-04
H13	Na17	1.0569396370E+01	1.1425934602E-04	5.6025952050E-03	5.5116508592E-04
H14	Na17	1.0569395843E+01	1.1425905450E-04	5.6025811897E-03	5.5116367968E-04
C15	Na17	6.2335164658E+01	4.1797201564E-05	3.4750734840E-04	2.0162165279E-04
H16	Na17	1.0614341797E+01	2.0767110392E-05	1.0139875483E-03	1.0017654207E-04

Benzene-NaAl$_4^-$ π-π

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)

Al1	Al2	1.7826573145E+02	9.5236931115E-01	3.5615904302E+00	3.5618892226E+00 (Bonded)
Al1	Al3	1.7826590413E+02	9.5207004849E-01	3.5604712730E+00	3.5607695124E+00 (Bonded)
Al2	Al3	1.7839185238E+02	6.7018567223E-01	2.5065141171E+00	2.5065137940E+00
Al1	Al4	1.7842148900E+02	6.7076743631E-01	2.5084794881E+00	2.5084800294E+00
Al2	Al4	1.7826584406E+02	9.5206694998E-01	3.5607583830E+00	3.5604604538E+00 (Bonded)
Al3	Al4	1.7826571645E+02	9.5236826017E-01	3.5618848328E+00	3.5615872685E+00 (Bonded)

Al1	C5	8.0359541505E+01	1.8131677457E-02	6.7807318189E-02	1.5081792709E-01
Al2	C5	8.0354451923E+01	1.4827250486E-02	5.5454352727E-02	1.2333195249E-01
Al3	C5	8.0341466717E+01	4.0818383135E-02	1.5266193327E-01	3.3952423576E-01 (Bonded)
Al4	C5	8.0362600480E+01	1.1979040210E-02	4.4798213972E-02	9.9640753994E-02
Al1	C6	8.0352733417E+01	4.1746571385E-02	1.5612030690E-01	3.4722323656E-01 (Bonded)
Al2	C6	8.0360826519E+01	1.2075937044E-02	4.5164359569E-02	1.0044048663E-01
Al3	C6	8.0358519121E+01	1.6711456224E-02	6.2501329523E-02	1.3899598757E-01
Al4	C6	8.0366154253E+01	1.4870209032E-02	5.5610365637E-02	1.2368158479E-01
C5	C6	3.5447583700E+01	1.3763301423E+00	1.1448210434E+01	1.1447498338E+01 (Bonded)
Al1	C7	8.0334497770E+01	2.9267454684E-02	1.0945195871E-01	2.4350349170E-01
Al2	C7	8.0326798502E+01	3.1185665149E-02	1.1663530449E-01	2.5946288930E-01
Al3	C7	8.0335520761E+01	1.3761863780E-02	5.1469768490E-02	1.1449789259E-01
Al4	C7	8.0342384155E+01	1.3460003055E-02	5.0336595118E-02	1.1198642921E-01
C5	C7	3.6088749347E+01	7.1990880207E-02	5.9881471796E-01	5.9895986482E-01
C6	C7	3.5439993337E+01	1.3739972072E+00	1.1428094367E+01	1.1431575487E+01 (Bonded)
Al1	C8	8.0362693680E+01	1.1979420321E-02	4.4799625814E-02	9.9643821450E-02
Al2	C8	8.0341531895E+01	4.0819384797E-02	1.5266569920E-01	3.3953224625E-01 (Bonded)
Al3	C8	8.0354538132E+01	1.4827632993E-02	5.5455776166E-02	1.2333501746E-01
Al4	C8	8.0359600061E+01	1.8131969420E-02	6.7808424681E-02	1.5082021291E-01
C5	C8	3.6085711043E+01	9.5648442005E-02	7.9559653469E-01	7.9559578189E-01
C6	C8	3.6099714743E+01	7.2136442248E-02	5.9998816956E-01	6.0002492430E-01
C7	C8	3.5438122791E+01	1.3733123558E+00	1.1425877564E+01	1.1423097905E+01 (Bonded)
Al1	C9	8.0366157149E+01	1.4870356820E-02	5.5610906321E-02	1.2368283612E-01
Al2	C9	8.0358494236E+01	1.6711755551E-02	6.2502457075E-02	1.3899850206E-01
Al3	C9	8.0360822318E+01	1.2076313841E-02	4.5165762978E-02	1.0044363857E-01
Al4	C9	8.0352701378E+01	4.1747208442E-02	1.5612272301E-01	3.4722859732E-01 (Bonded)
C5	C9	3.6099674187E+01	7.2136242559E-02	6.0002383105E-01	5.9998661599E-01
C6	C9	3.6090088160E+01	9.5803971908E-02	7.9684065295E-01	7.9684079547E-01
C7	C9	3.6090990116E+01	7.1990725005E-02	5.9895857354E-01	5.9877628700E-01
C8	C9	3.5447611227E+01	1.3763305461E+00	1.1448202961E+01	1.1447503745E+01 (Bonded)
Al1	C10	8.0342406387E+01	1.3459756323E-02	5.0335661548E-02	1.1198436977E-01
Al2	C10	8.0335515308E+01	1.3761587864E-02	5.1468743191E-02	1.1449559019E-01
Al3	C10	8.0326813887E+01	3.1185148144E-02	1.1663335584E-01	2.5945857245E-01
Al4	C10	8.0334485690E+01	2.9266468562E-02	1.0944829451E-01	2.4349527277E-01
C5	C10	3.5438091126E+01	1.3733116106E+00	1.1423102515E+01	1.1425870686E+01 (Bonded)
C6	C10	3.6090998723E+01	7.1990722294E-02	5.9877615736E-01	5.9895851545E-01
C7	C10	3.6068887982E+01	9.4209568317E-02	7.8381803558E-01	7.8381798907E-01
C8	C10	3.6088785614E+01	7.1990996672E-02	5.9881512010E-01	5.9896079826E-01
C9	C10	3.5439989088E+01	1.3739970696E+00	1.1428095267E+01	1.1431573665E+01 (Bonded)
Al1	H11	1.3479436809E+01	3.2865291981E-03	1.2290684720E-02	1.6297246410E-01
Al2	H11	1.3477916262E+01	4.0658773566E-03	1.5206500847E-02	2.0161879345E-01
Al3	H11	1.3473540737E+01	1.2820403560E-02	4.7948680042E-02	6.3573838327E-01
Al4	H11	1.3480006211E+01	2.1419054258E-03	8.0101189990E-03	1.0621284160E-01
C5	H11	5.5798074699E+00	9.6249685006E-01	8.0059762869E+00	4.7728309683E+01 (Bonded)
C6	H11	6.0366689608E+00	4.9527928732E-02	4.1194395476E-01	2.4559917472E+00
C7	H11	6.0545079562E+00	1.0158307612E-02	8.4516518435E-02	5.0373032550E-01
C8	H11	6.0582661024E+00	5.5910550858E-03	4.6505930984E-02	2.7724933185E-01
C9	H11	6.0563680837E+00	1.0127514595E-02	8.4234678641E-02	5.0220336086E-01
C10	H11	6.0349522068E+00	4.9270525508E-02	4.0992783338E-01	2.4432276319E+00
Al1	H12	1.3475526616E+01	1.3396453393E-02	5.0098926586E-02	6.6424714621E-01
Al2	H12	1.3480045128E+01	2.0974903371E-03	7.8446755255E-03	1.0400155398E-01
Al3	H12	1.3479628816E+01	2.9335913911E-03	1.0971716634E-02	1.4545862644E-01
Al4	H12	1.3480145471E+01	4.1529241082E-03	1.5530758688E-02	2.0591778335E-01
C5	H12	6.0368326146E+00	4.9475930402E-02	4.1153706170E-01	2.4532049351E+00
C6	H12	5.5807639806E+00	9.6236732292E-01	8.0044009731E+00	4.7717834648E+01 (Bonded)
C7	H12	6.0354354013E+00	4.9332537772E-02	4.1044379607E-01	2.4460949827E+00
C8	H12	6.0565086260E+00	1.0135378754E-02	8.4305237136E-02	5.0255065397E-01
C9	H12	6.0591421525E+00	5.6088106205E-03	4.6650770604E-02	2.7810617774E-01
C10	H12	6.0550266319E+00	1.0150795714E-02	8.4454014872E-02	5.0331508549E-01
H11	H12	1.0134456904E+00	6.6518410907E-03	3.2985160577E-01	3.2982359823E-01
Al1	H13	1.3464411689E+01	7.1181555296E-03	2.6619877729E-02	3.5331878903E-01
Al2	H13	1.3462863040E+01	7.9559062664E-03	2.9755323334E-02	3.9490162247E-01
Al3	H13	1.3465216570E+01	3.2523186044E-03	1.2163765628E-02	1.6143300973E-01
Al4	H13	1.3466430955E+01	3.0738109870E-03	1.1495181575E-02	1.5257255494E-01
C5	H13	6.0500893545E+00	1.0145265391E-02	8.4387553203E-02	5.0357327363E-01
C6	H13	6.0308919037E+00	4.9293494326E-02	4.0999406833E-01	2.4467458810E+00

C7	H13	5.5722457545E+00	9.6289775227E-01	8.0112523402E+00	4.7794666242E+01	(Bonded)
C8	H13	6.0305245559E+00	4.9286321683E-02	4.0995952275E-01	2.4463898577E+00	
C9	H13	6.0504708899E+00	1.0133355722E-02	8.4283261678E-02	5.0298212192E-01	
C10	H13	6.0509674876E+00	5.4550043847E-03	4.5385311105E-02	2.7076614656E-01	
H11	H13	1.0147655091E+00	1.8622411283E-03	9.2344843798E-02	9.2434729417E-02	
H12	H13	1.0124746808E+00	6.6163969165E-03	3.2806614118E-01	3.2841335604E-01	
Al1	H14	1.3479850053E+01	2.1417921540E-03	8.0096936659E-03	1.0620847831E-01	
Al2	H14	1.3473380207E+01	1.2819765534E-02	4.7946299991E-02	6.3571424854E-01	
Al3	H14	1.3477758982E+01	4.0656898384E-03	1.5205797564E-02	2.0161187453E-01	
Al4	H14	1.3479274853E+01	3.2863728255E-03	1.2290102584E-02	1.6296663348E-01	
C5	H14	6.0581889141E+00	5.5908778366E-03	4.6504500643E-02	2.7724381487E-01	
C6	H14	6.0562977125E+00	1.0127332616E-02	8.4233149978E-02	5.0220026460E-01	
C7	H14	6.0348811878E+00	4.9268795264E-02	4.0991346218E-01	2.4431706706E+00	
C8	H14	5.5797454685E+00	9.6248923906E-01	8.0059054038E+00	4.7728495633E+01	(Bonded)
C9	H14	6.0365972876E+00	4.9526014094E-02	4.1192810361E-01	2.4559257927E+00	
C10	H14	6.0544368988E+00	1.0158092512E-02	8.4514723797E-02	5.0372560483E-01	
H11	H14	1.0164656710E+00	4.1521172505E-04	2.0589525873E-02	2.0589768905E-02	
H12	H14	1.0158242651E+00	1.8706887038E-03	9.2755865792E-02	9.2764837267E-02	
H13	H14	1.0123839126E+00	6.6014564269E-03	3.2767176566E-01	3.2735699420E-01	
Al1	H15	1.3480239739E+01	4.1530007481E-03	1.5531041948E-02	2.0592018749E-01	
Al2	H15	1.3479718471E+01	2.9335829153E-03	1.0971686349E-02	1.4545722011E-01	
Al3	H15	1.3480138234E+01	2.0975344997E-03	7.8448396835E-03	1.0400303868E-01	
Al4	H15	1.3475614992E+01	1.3396675553E-02	5.0099768215E-02	6.6425365873E-01	
C5	H15	6.0565439384E+00	1.0135466809E-02	8.4306049341E-02	5.0255161322E-01	
C6	H15	6.0591842907E+00	5.6088916996E-03	4.6651436628E-02	2.7810831263E-01	
C7	H15	6.0550672833E+00	1.0150937765E-02	8.4455201743E-02	5.0331871690E-01	
C8	H15	6.0368788035E+00	4.9477207718E-02	4.1154729690E-01	2.4532516385E+00	
C9	H15	5.5808017685E+00	9.6237176758E-01	8.0044393729E+00	4.7717731548E+01	(Bonded)
C10	H15	6.0354764066E+00	4.9333410269E-02	4.1045103084E-01	2.4461216620E+00	
H11	H15	1.0158431383E+00	1.8707307512E-03	9.2765827362E-02	9.2757321851E-02	
H12	H15	1.0166564771E+00	4.1673619124E-04	2.0663366463E-02	2.0663226385E-02	
H13	H15	1.0148590395E+00	1.8614516393E-03	9.2395542120E-02	9.2297231286E-02	
H14	H15	1.0134406206E+00	6.6517631558E-03	3.2985163455E-01	3.2981749806E-01	
Al1	H16	1.3466344863E+01	3.0738199958E-03	1.1495212785E-02	1.5257401028E-01	
Al2	H16	1.3465125883E+01	3.2522480306E-03	1.2163503248E-02	1.6143057340E-01	
Al3	H16	1.3462775870E+01	7.9557475908E-03	2.9754726047E-02	3.9489635580E-01	
Al4	H16	1.3464319769E+01	7.1181950684E-03	2.6620031337E-02	3.5332308627E-01	
C5	H16	6.0304792771E+00	4.9285397891E-02	4.0995222663E-01	2.4463601691E+00	
C6	H16	6.0504319900E+00	1.0133294335E-02	8.4282736024E-02	5.0298239850E-01	
C7	H16	6.0509271632E+00	5.4549317963E-03	4.5384709867E-02	2.7076433269E-01	
C8	H16	6.0500551394E+00	1.0145132208E-02	8.4386365554E-02	5.0356999043E-01	
C9	H16	6.0308513823E+00	4.9292343611E-02	4.0998457070E-01	2.4467049311E+00	
C10	H16	5.5722085090E+00	9.6289295864E-01	8.0112119821E+00	4.7794744121E+01	(Bonded)
H11	H16	1.0123891003E+00	6.6016357140E-03	3.2736202072E-01	3.2768283005E-01	
H12	H16	1.0148454545E+00	1.8614252636E-03	9.2296549167E-02	9.2394843450E-02	
H13	H16	1.0144984447E+00	4.0758723146E-04	2.0231115553E-02	2.0231249237E-02	
H14	H16	1.0147468269E+00	1.8622049709E-03	9.2344140811E-02	9.2433545478E-02	
H15	H16	1.0124750067E+00	6.6160930622E-03	3.2804885105E-01	3.2840044384E-01	
Al1	Na17	1.3905156336E+02	1.7666424396E-01	6.6067404032E-01	8.4878639887E-01	
Al2	Na17	1.3903991811E+02	1.7661098180E-01	6.6053026416E-01	8.4853049987E-01	
Al3	Na17	1.3903993580E+02	1.7661148043E-01	6.6053204389E-01	8.4853289555E-01	(Bonded)
Al4	Na17	1.3905153324E+02	1.7666441756E-01	6.6067483211E-01	8.4878723292E-01	
C5	Na17	6.2555015420E+01	3.7848369198E-03	3.1481988359E-02	1.8184314083E-02	
C6	Na17	6.2558904374E+01	3.7896794443E-03	3.1520307381E-02	1.8207580075E-02	
C7	Na17	6.2539860899E+01	3.7748585371E-03	3.1406599733E-02	1.8136372772E-02	
C8	Na17	6.2555074551E+01	3.7849600175E-03	3.1482982487E-02	1.8184905508E-02	
C9	Na17	6.2558893147E+01	3.7897555319E-03	3.1520945870E-02	1.8207945639E-02	
C10	Na17	6.2539864649E+01	3.7747806022E-03	3.1405949455E-02	1.8135998332E-02	
H11	Na17	1.0493115913E+01	4.3726347740E-04	2.1683028533E-02	2.1008398984E-03	
H12	Na17	1.0494004566E+01	4.4207582497E-04	2.1919801946E-02	2.1239609051E-03	
H13	Na17	1.0482918370E+01	4.2443667207E-04	2.1067459171E-02	2.0392132915E-03	
H14	Na17	1.0492992063E+01	4.3724485371E-04	2.1682360949E-02	2.1007504206E-03	
H15	Na17	1.0494075706E+01	4.4207864320E-04	2.1919793088E-02	2.1239744453E-03	
H16	Na17	1.0482849102E+01	4.2443231827E-04	2.1067382274E-02	2.0391923736E-03	

Benzene-KAl$_4^-$ CH-π

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7902362937E+02	9.8609866018E-01	3.6806646152E+00	3.6791686456E+00 (Bonded)
Al1	Al3	1.7902268921E+02	9.8795628154E-01	3.6875982837E+00	3.6860997290E+00 (Bonded)
Al2	Al3	1.7923491370E+02	7.0949217545E-01	2.6471401612E+00	2.6471403285E+00
Al1	Al4	1.7909114212E+02	7.0517641742E-01	2.6321077108E+00	2.6321074997E+00
Al2	Al4	1.7902271404E+02	9.8795813955E-01	3.6861064283E+00	3.6876049230E+00 (Bonded)
Al3	Al4	1.7902363303E+02	9.8609745923E-01	3.6791643974E+00	3.6806598373E+00 (Bonded)
Al1	H5	1.2842369632E+01	2.8446262365E-02	1.0617715605E-01	1.4819496720E+00
Al2	H5	1.2847686324E+01	2.8267996503E-02	1.0546888522E-01	1.4726626510E+00 (Bonded)
Al3	H5	1.2847685613E+01	2.8267791567E-02	1.0546812727E-01	1.4726519746E+00
Al4	H5	1.2842370660E+01	2.8446269248E-02	1.0617717322E-01	1.4819500306E+00
Al1	C6	8.0538093663E+01	1.2535985970E-02	4.6791220635E-02	1.0424554036E-01
Al2	C6	8.0571326412E+01	1.1570019770E-02	4.3168149078E-02	9.6212852011E-02
Al3	C6	8.0571321356E+01	1.1569943840E-02	4.3167868509E-02	9.6212220599E-02
Al4	C6	8.0538100169E+01	1.2535895465E-02	4.6790879067E-02	1.0424478775E-01
H5	C6	5.3130528258E+00	9.1540809560E-01	4.7689524537E+01	7.6122621551E+00 (Bonded)
Al1	C7	8.0419432501E+01	3.5489699470E-03	1.3246715194E-02	2.9557375316E-02
Al2	C7	8.0451840789E+01	4.1317744433E-03	1.5415795190E-02	3.4411226290E-02
Al3	C7	8.0452821917E+01	2.1593467450E-03	8.0565988602E-03	1.7983984969E-02
Al4	C7	8.0420022638E+01	2.3815987703E-03	8.8894407551E-03	1.9834997128E-02
H5	C7	5.7402806077E+00	4.3305221920E-02	2.2560489177E+00	3.6066484545E-01
C6	C7	3.5404074837E+01	1.3869087762E+00	1.1533121938E+01	1.1550783421E+01 (Bonded)
Al1	C8	8.0420051322E+01	2.3814783041E-03	8.8889918217E-03	1.9833985183E-02
Al2	C8	8.0452862156E+01	2.1592195498E-03	8.0561237808E-03	1.7982917788E-02
Al3	C8	8.0451870994E+01	4.1313708451E-03	1.5414290326E-02	3.4407849941E-02
Al4	C8	8.0419474048E+01	3.5489279988E-03	1.3246557557E-02	2.9557013063E-02
H5	C8	5.7402831331E+00	4.3305197153E-02	2.2560476274E+00	3.6066448188E-01
C6	C8	3.5404090475E+01	1.3869089884E+00	1.1533123703E+01	1.1550780151E+01 (Bonded)
C7	C8	3.6003569851E+01	7.7561845425E-02	6.4596900219E-01	6.4596872045E-01
Al1	H9	1.3318683361E+01	4.8590623326E-03	1.8136703266E-02	2.4431272786E-01
Al2	H9	1.3322551757E+01	7.9551411631E-03	2.9680910360E-02	3.9998298129E-01
Al3	H9	1.3324837677E+01	3.3816167649E-03	1.2616931411E-02	1.7002704634E-01
Al4	H9	1.3319669636E+01	2.8886494036E-03	1.0782033504E-02	1.4524074138E-01
H5	H9	9.5127181902E-01	6.2902569302E-03	3.2770014124E-01	3.1627291941E-01
C6	H9	5.9551314403E+00	4.8256021861E-02	4.0128276201E-01	2.4263035807E+00
C7	H9	5.4904879525E+00	9.5925807446E-01	7.9891211691E+00	4.8231313132E+01 (Bonded)
C8	H9	5.9650656066E+00	1.0107973996E-02	8.4183595587E-02	5.0822700573E-01
Al1	H10	1.3319629722E+01	2.8886127635E-03	1.0781897608E-02	1.4523932285E-01
Al2	H10	1.3324799661E+01	3.3815754340E-03	1.2616776406E-02	1.7002546427E-01
Al3	H10	1.3322512075E+01	7.9550618321E-03	2.9680616250E-02	3.9998015945E-01
Al4	H10	1.3318645602E+01	4.8589900375E-03	1.8136431966E-02	2.4430980563E-01
H5	H10	9.5126906664E-01	6.2901927738E-03	3.2769679892E-01	3.1627061634E-01
C6	H10	5.9551141893E+00	4.8255635573E-02	4.0127954976E-01	2.4262912368E+00
C7	H10	5.9650455992E+00	1.0107946166E-02	8.4183400523E-02	5.0822708916E-01
C8	H10	5.4904733132E+00	9.5925772587E-01	7.9891147815E+00	4.8231436317E+01 (Bonded)
H9	H10	9.8804666745E-01	1.7026560354E-03	8.5609220904E-02	8.5609470664E-02
Al1	C11	8.0521695045E+01	5.4844164159E-04	2.0470869957E-03	4.5619462700E-03
Al2	C11	8.0554391975E+01	6.3590400538E-04	2.3725801207E-03	5.2894595986E-03
Al3	C11	8.0554427986E+01	5.5369749006E-04	2.0658648629E-03	4.6056645008E-03
Al4	C11	8.0521693222E+01	5.6500745839E-04	2.1089196006E-03	4.6997409967E-03
H5	C11	5.7647194310E+00	8.8661929085E-03	4.6189729619E-01	7.3749133181E-02
C6	C11	3.6105213574E+01	7.5086781115E-02	6.2439939627E-01	6.2457303577E-01
C7	C11	3.5392314656E+01	1.3903579652E+00	1.1579509777E+01	1.1565019598E+01 (Bonded)
C8	C11	3.6035964753E+01	1.0308925004E-01	8.5857202821E-01	8.5749801622E-01
H9	C11	5.9528150357E+00	4.9564205794E-02	2.4920788195E+00	4.1227584960E-01
H10	C11	5.9747466122E+00	5.6661743068E-03	2.8489499523E-01	4.7131327717E-02
Al1	C12	8.0521693777E+01	5.6501115360E-04	2.1089335623E-03	4.6997713240E-03
Al2	C12	8.0554440097E+01	5.5369999647E-04	2.0658740837E-03	4.6056849478E-03
Al3	C12	8.0554393903E+01	6.3590332899E-04	2.3725777471E-03	5.2894535115E-03
Al4	C12	8.0521708521E+01	5.4844169874E-04	2.0470870448E-03	4.5619463478E-03
H5	C12	5.7647199337E+00	8.8661929932E-03	4.6189730060E-01	7.3749127459E-02
C6	C12	3.6105216722E+01	7.5086784352E-02	6.2439942319E-01	6.2457300827E-01

C7	C12	3.6035952171E+01	1.0308922424E-01	8.5857218787E-01	8.5749772696E-01	
C8	C12	3.5392333316E+01	1.3903584133E+00	1.1579508459E+01	1.1565022317E+01	(Bonded)
H9	C12	5.9747645271E+00	5.6662647081E-03	2.8489870943E-01	4.7132075570E-02	
H10	C12	5.9527982484E+00	4.9563943657E-02	2.4920729098E+00	4.1227363322E-01	
C11	C12	3.6095476472E+01	7.4470959748E-02	6.1945062387E-01	6.1945056989E-01	
Al1	H13	1.3683259747E+01	2.7995856983E-04	1.0449599450E-03	1.3703575082E-02	
Al2	H13	1.3688813218E+01	3.0050303199E-04	1.1211873394E-03	1.4709197378E-02	
Al3	H13	1.3688810544E+01	3.0412000208E-04	1.1346824533E-03	1.4886242936E-02	
Al4	H13	1.3683259096E+01	2.8345600693E-04	1.0580142263E-03	1.3874769669E-02	
H5	H13	9.7955743772E-01	1.6325041092E-03	8.5047690911E-02	7.9908761662E-02	
C6	H13	6.1365947226E+00	1.0558586926E-02	8.7802076530E-02	5.1682786058E-01	
C7	H13	6.1068242344E+00	5.1317355722E-02	4.2739340315E-01	2.5119118074E+00	
C8	H13	6.1292654323E+00	6.4403090830E-03	5.3637689961E-02	3.1524399887E-01	
H9	H13	1.0125083286E+00	6.5742688117E-03	3.3055298268E-01	3.2180113767E-01	
H10	H13	1.0155619245E+00	4.6115001760E-04	2.3186602627E-02	2.2572639566E-02	
C11	H13	5.6550674070E+00	9.7019817502E-01	8.0701238017E+00	4.7489825170E+01	(Bonded)
C12	H13	6.1348783366E+00	1.0577386061E-02	8.7982857283E-02	5.1774805158E-01	
Al1	H14	1.3683257626E+01	2.8345611840E-04	1.0580147272E-03	1.3874775504E-02	
Al2	H14	1.3688811037E+01	3.0411942734E-04	1.1346802371E-03	1.4886215208E-02	
Al3	H14	1.3688811980E+01	3.0050256870E-04	1.1211856818E-03	1.4709175101E-02	
Al4	H14	1.3683260473E+01	2.7995732606E-04	1.0449552187E-03	1.3703514574E-02	
H5	H14	9.7955741093E-01	1.6325043099E-03	8.5047701368E-02	7.9908773662E-02	
C6	H14	6.1365945565E+00	1.0558584935E-02	8.7802059975E-02	5.1682777720E-01	
C7	H14	6.1292625937E+00	6.4403032340E-03	5.3637664641E-02	3.1524372115E-01	
C8	H14	6.1068267329E+00	5.1317374075E-02	4.2739336959E-01	2.5119127742E+00	
H9	H14	1.0155648578E+00	4.6115505587E-04	2.3186788304E-02	2.2572886797E-02	
H10	H14	1.0125053450E+00	6.5742537225E-03	3.3055318836E-01	3.2180040783E-01	
C11	H14	6.1348776366E+00	1.0577381717E-02	8.7982828821E-02	5.1774785307E-01	
C12	H14	5.6550676537E+00	9.7019841747E-01	8.0701251151E+00	4.7489838329E+01	(Bonded)
H13	H14	1.0424282505E+00	1.9864067918E-03	9.7231796232E-02	9.7231798878E-02	
Al1	C15	8.0575579695E+01	5.1989706620E-04	1.9405428811E-03	4.3216208117E-03	
Al2	C15	8.0608405245E+01	3.9392844013E-04	1.4697608100E-03	3.2745123138E-03	
Al3	C15	8.0608400149E+01	3.9392798736E-04	1.4697592136E-03	3.2745085501E-03	
Al4	C15	8.0575586159E+01	5.1989640096E-04	1.9405402424E-03	4.3216152818E-03	
H5	C15	5.7706270685E+00	4.7702131268E-03	2.4851123455E-01	3.9652180527E-02	
C6	C15	3.6115082910E+01	1.0370817779E-01	8.6240644006E-01	8.6206952990E-01	
C7	C15	3.6074516000E+01	7.4241401845E-02	6.1831489449E-01	6.1712828972E-01	
C8	C15	3.6074531740E+01	7.4241421417E-02	6.1831478783E-01	6.1712845242E-01	
H9	C15	5.9765952938E+00	1.0001889837E-02	5.0289311448E-01	8.3140256191E-02	
H10	C15	5.9765778647E+00	1.0001846155E-02	5.0289238530E-01	8.3139893084E-02	
C11	C15	3.5462088583E+01	1.3895870646E+00	1.1558607235E+01	1.1550879527E+01	(Bonded)
C12	C15	3.5462091701E+01	1.3895871307E+00	1.1558606777E+01	1.1550880076E+01	(Bonded)
H13	C15	6.1181605616E+00	5.2227588549E-02	2.5564664138E+00	4.3413946392E-01	
H14	C15	6.1181603821E+00	5.2227613133E-02	2.5564676867E+00	4.3413966827E-01	
Al1	H16	1.3741011097E+01	1.2453672868E-04	4.6483982694E-04	6.0703107860E-03	
Al2	H16	1.3746597026E+01	1.2706430548E-04	4.7408137500E-04	6.1935128076E-03	
Al3	H16	1.3746596157E+01	1.2706431087E-04	4.7408142507E-04	6.1935130702E-03	
Al4	H16	1.3741012199E+01	1.2453648051E-04	4.6483886335E-04	6.0702986896E-03	
H5	H16	9.8431356479E-01	3.8452915055E-04	2.0032608897E-02	1.8743156938E-02	
C6	H16	6.1644405287E+00	6.6412749687E-03	5.5226872418E-02	3.2371657344E-01	
C7	H16	6.1530373712E+00	1.0586217794E-02	8.8166656017E-02	5.1600546074E-01	
C8	H16	6.1530400511E+00	1.0586229704E-02	8.8166716749E-02	5.1600604123E-01	
H9	H16	1.0191178445E+00	1.9181118379E-03	9.6442297580E-02	9.3494787455E-02	
H10	H16	1.0191148707E+00	1.9181075329E-03	9.6442362490E-02	9.3494577616E-02	
C11	H16	6.1399783033E+00	5.2136288563E-02	4.3367047485E-01	2.5412862387E+00	
C12	H16	6.1399788777E+00	5.2136214486E-02	4.3366982089E-01	2.5412826280E+00	
H13	H16	1.0443663864E+00	6.9059465243E-03	3.3803629146E-01	3.3661749525E-01	
H14	H16	1.0443663632E+00	6.9059358199E-03	3.3803577670E-01	3.3661697348E-01	
C15	H16	5.6843616200E+00	9.7162000616E-01	8.0765472872E+00	4.7359806749E+01	(Bonded)
Al1	K17	2.4543736689E+02	1.7029287705E-01	6.3562703419E-01	4.6455730441E-01	
Al2	K17	2.4553642440E+02	1.7183937025E-01	6.4113871021E-01	4.6877612275E-01	(Bonded)
Al3	K17	2.4553640899E+02	1.7183913265E-01	6.4113786423E-01	4.6877547457E-01	
Al4	K17	2.4543738650E+02	1.7029304695E-01	6.3562761734E-01	4.6455776788E-01	
H5	K17	1.7587172986E+01	7.5265338727E-03	3.9210579798E-01	2.0532310851E-02	
C6	K17	1.1020195508E+02	4.5226917221E-03	3.7609362645E-02	1.2337858820E-02	
C7	K17	1.1003540041E+02	6.2115028939E-04	5.1732115249E-03	1.6944919193E-03	

C8	K17	1.1003544842E+02	6.2110722753E-04	5.1728506308E-03	1.6943744469E-03
H9	K17	1.8225976603E+01	1.0716396062E-03	5.3881835124E-02	2.9234223730E-03
H10	K17	1.8225923435E+01	1.0716258695E-03	5.3881301644E-02	2.9233848996E-03
C11	K17	1.1017351570E+02	1.2503123254E-04	1.0400117746E-03	3.4108398051E-04
C12	K17	1.1017352530E+02	1.2503161791E-04	1.0400148894E-03	3.4108503178E-04
H13	K17	1.8722139515E+01	1.3828244798E-04	6.7687297786E-03	3.7723316671E-04
H14	K17	1.8722139005E+01	1.3828225554E-04	6.7687205431E-03	3.7723264174E-04
C15	K17	1.1024726132E+02	4.9252466382E-05	4.0940889568E-04	1.3436024697E-04
H16	K17	1.8801102008E+01	3.6338074723E-05	1.7712317424E-03	9.9129912730E-05

Benzene-KAl$_4^-$ π-π

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7855669667E+02	9.6355899873E-01	3.6006322106E+00	3.6005719753E+00 (Bonded)
Al1	Al3	1.7855677786E+02	9.6345146034E-01	3.6002303606E+00	3.6001695807E+00 (Bonded)
Al2	Al3	1.7870171706E+02	6.7956345928E-01	2.5393537398E+00	2.5393533509E+00
Al1	Al4	1.7869588691E+02	6.7908860373E-01	2.5376217789E+00	2.5376224849E+00
Al2	Al4	1.7855670186E+02	9.6344899875E-01	3.6001609337E+00	3.6002221636E+00 (Bonded)
Al3	Al4	1.7855667514E+02	9.6355727948E-01	3.6005649995E+00	3.6006267877E+00 (Bonded)
Al1	C5	8.0401043610E+01	1.6071455068E-02	6.0055895762E-02	1.3371793676E-01
Al2	C5	8.0403512859E+01	1.3823345206E-02	5.1654283150E-02	1.1501318283E-01
Al3	C5	8.0392222869E+01	3.6427954845E-02	1.3612187050E-01	3.0308836018E-01 (Bonded)
Al4	C5	8.0403398091E+01	1.1317756132E-02	4.2292260952E-02	9.4166146892E-02
Al1	C6	8.0391407051E+01	3.6490697491E-02	1.3635862562E-01	3.0360822863E-01 (Bonded)
Al2	C6	8.0405323827E+01	1.1347551560E-02	4.2402879521E-02	9.4413378346E-02
Al3	C6	8.0403094727E+01	1.5830380180E-02	5.9154047214E-02	1.3171120355E-01
Al4	C6	8.0402714881E+01	1.3830300173E-02	5.1681151027E-02	1.1507022955E-01
C5	C6	3.5425028507E+01	1.3777056900E+00	1.1462805425E+01	1.1462723732E+01 (Bonded)
Al1	C7	8.0375879951E+01	2.6657123679E-02	9.9612476546E-02	2.2184778260E-01
Al2	C7	8.0377040870E+01	2.7025009143E-02	1.0098550341E-01	2.2490942479E-01
Al3	C7	8.0384228008E+01	1.2675356416E-02	4.7364537262E-02	1.0548773935E-01
Al4	C7	8.0382876486E+01	1.2619327879E-02	4.7155982288E-02	1.0502145474E-01
C5	C7	3.6068465036E+01	7.2468963596E-02	6.0295724626E-01	6.0310628688E-01
C6	C7	3.5416962883E+01	1.3759878951E+00	1.1448431413E+01	1.1451342879E+01 (Bonded)
Al1	C8	8.0403412735E+01	1.1317738369E-02	4.2292182809E-02	9.4166008157E-02
Al2	C8	8.0392202844E+01	3.6427907005E-02	1.3612171258E-01	3.0308799130E-01 (Bonded)
Al3	C8	8.0403517491E+01	1.3823242400E-02	5.1653891081E-02	1.1501233852E-01
Al4	C8	8.0401013631E+01	1.6071208097E-02	6.0054989586E-02	1.3371589477E-01
C5	C8	3.6065044273E+01	9.7152461148E-02	8.0832921480E-01	8.0832929255E-01
C6	C8	3.6077556530E+01	7.2642696849E-02	6.0439843657E-01	6.0440280214E-01
C7	C8	3.5416871774E+01	1.3756485435E+00	1.1448518703E+01	1.1445690627E+01 (Bonded)
Al1	C9	8.0402743024E+01	1.3830306268E-02	5.1681159429E-02	1.1507027200E-01
Al2	C9	8.0403088199E+01	1.5830363298E-02	5.9153993191E-02	1.3171105363E-01
Al3	C9	8.0405341858E+01	1.1347674400E-02	4.2403332048E-02	9.4414393608E-02
Al4	C9	8.0391390429E+01	3.6490759228E-02	1.3635889425E-01	3.0360872047E-01 (Bonded)
C5	C9	3.6077562523E+01	7.2642847764E-02	6.0440399966E-01	6.0439964877E-01
C6	C9	3.6065589188E+01	9.7104274122E-02	8.0792253054E-01	8.0792247248E-01
C7	C9	3.6068726535E+01	7.2465779318E-02	6.0307978646E-01	6.0292641211E-01
C8	C9	3.5425027694E+01	1.3777055603E+00	1.1462805448E+01	1.1462721829E+01 (Bonded)
Al1	C10	8.0382943238E+01	1.2619518021E-02	4.7156679692E-02	1.0502297903E-01
Al2	C10	8.0384260017E+01	1.2675685662E-02	4.7365774822E-02	1.0549042105E-01
Al3	C10	8.0377097120E+01	2.7026101671E-02	1.0098957044E-01	2.2491839264E-01
Al4	C10	8.0375901978E+01	2.6657312766E-02	9.9613210836E-02	2.2184923347E-01
C5	C10	3.5416894864E+01	1.3756492668E+00	1.1445695545E+01	1.1448518388E+01 (Bonded)
C6	C10	3.6068743894E+01	7.2465831761E-02	6.0292689177E-01	6.0307988919E-01
C7	C10	3.6047879642E+01	9.5835195196E-02	7.9756637683E-01	7.9756593548E-01
C8	C10	3.6068481489E+01	7.2469071921E-02	6.0295820554E-01	6.0310685466E-01
C9	C10	3.5416985102E+01	1.3759886040E+00	1.1448436489E+01	1.1451342442E+01 (Bonded)
Al1	H11	1.3512231584E+01	3.1477714212E-03	1.1762608398E-02	1.5583502792E-01
Al2	H11	1.3512046283E+01	3.9705277635E-03	1.4836840309E-02	1.9656678395E-01
Al3	H11	1.3508055577E+01	1.1956079178E-02	4.4676783763E-02	5.9190318583E-01
Al4	H11	1.3512687083E+01	2.2292548936E-03	8.3302934422E-03	1.1036252386E-01
C5	H11	5.5879039613E+00	9.6293295707E-01	8.0118077494E+00	4.7671404358E+01 (Bonded)
C6	H11	6.0445481837E+00	4.9731022923E-02	4.1376977738E-01	2.4620070230E+00

C7	H11	6.0627769982E+00	1.0187137425E-02	8.4780108911E-02	5.0432913722E-01
C8	H11	6.0664940011E+00	5.7517098849E-03	4.7855458599E-02	2.8474680990E-01
C9	H11	6.0643284004E+00	1.0171461816E-02	8.4628124289E-02	5.0355309329E-01
C10	H11	6.0431146450E+00	4.9518559395E-02	4.1210659682E-01	2.4514887052E+00
Al1	H12	1.3509132829E+01	1.2026394218E-02	4.4940291622E-02	5.9532517901E-01
Al2	H12	1.3514260637E+01	2.2229796760E-03	8.3067028938E-03	1.1004094408E-01
Al3	H12	1.3513832796E+01	3.0827997534E-03	1.1519627456E-02	1.5260337237E-01
Al4	H12	1.3513154687E+01	3.9751597992E-03	1.4854401667E-02	1.9677657960E-01
C5	H12	6.0451214256E+00	4.9702180241E-02	4.1353274898E-01	2.4603350608E+00
C6	H12	5.5885610278E+00	9.6290949509E-01	8.0115554437E+00	4.7665514464E+01 (Bonded)
C7	H12	6.0436871038E+00	4.9570780528E-02	4.1254142323E-01	2.4538305711E+00
C8	H12	6.0648818926E+00	1.0180078463E-02	8.4700433988E-02	5.0392968364E-01
C9	H12	6.0671403703E+00	5.7516823460E-03	4.7854880374E-02	2.8471720287E-01
C10	H12	6.0633808702E+00	1.0189963741E-02	8.4803583348E-02	5.0441902022E-01
H11	H12	1.0167900679E+00	6.6976153206E-03	3.3157524191E-01	3.3154235322E-01
Al1	H13	1.3500685145E+01	6.9564797648E-03	2.5995009280E-02	3.4463660263E-01
Al2	H13	1.3500830404E+01	7.1177943304E-03	2.6597365419E-02	3.5262841828E-01
Al3	H13	1.3502825780E+01	3.1311797556E-03	1.1700411045E-02	1.5512431426E-01
Al4	H13	1.3502612136E+01	3.0949857683E-03	1.1565361917E-02	1.5333119860E-01
C5	H13	6.0599493778E+00	1.0181146778E-02	8.4709314448E-02	5.0439244489E-01
C6	H13	6.0403079842E+00	4.9550382844E-02	4.1226682407E-01	2.4548156797E+00
C7	H13	5.5818833702E+00	9.6331555650E-01	8.0169722258E+00	4.7724396804E+01 (Bonded)
C8	H13	6.0402565708E+00	4.9565594077E-02	4.1239636260E-01	2.4555692717E+00
C9	H13	6.0599947879E+00	1.0177647040E-02	8.4679586302E-02	5.0421906155E-01
C10	H13	6.0607293643E+00	5.6302790147E-03	4.6856676612E-02	2.7893421631E-01
H11	H13	1.0183723532E+00	1.8750798297E-03	9.2828569332E-02	9.2894849698E-02
H12	H13	1.0160783612E+00	6.6652929368E-03	3.2994234506E-01	3.3021067996E-01
Al1	H14	1.3512681413E+01	2.2292405450E-03	8.3302375073E-03	1.1036189057E-01
Al2	H14	1.3508044150E+01	1.1955921389E-02	4.4676200990E-02	5.9189578756E-01
Al3	H14	1.3512038939E+01	3.9704825120E-03	1.4836668943E-02	1.9656468096E-01
Al4	H14	1.3512218370E+01	3.1478092042E-03	1.1762752858E-02	1.5583700723E-01
C5	H14	6.0664903447E+00	5.7517145176E-03	4.7855492541E-02	2.8474723807E-01
C6	H14	6.0643237216E+00	1.0171471286E-02	8.4628209158E-02	5.0355391369E-01
C7	H14	6.0431071041E+00	4.9518452058E-02	4.1210593157E-01	2.4514851031E+00
C8	H14	5.5878994587E+00	9.6293231900E-01	8.0118032111E+00	4.7671406056E+01 (Bonded)
C9	H14	6.0445443555E+00	4.9731075740E-02	4.1377018710E-01	2.4620113568E+00
C10	H14	6.0627761221E+00	1.0187131434E-02	8.4780012137E-02	5.0432919276E-01
H11	H14	1.0198216793E+00	4.3059459193E-04	2.1317215031E-02	2.1317229916E-02
H12	H14	1.0191957839E+00	1.8847587471E-03	9.3298483167E-02	9.3307803441E-02
H13	H14	1.0159814009E+00	6.6555609525E-03	3.2972853984E-01	3.2949350898E-01
Al1	H15	1.3513175417E+01	3.9753008430E-03	1.4854924588E-02	1.9678331336E-01
Al2	H15	1.3513847684E+01	3.0829684234E-03	1.1520259497E-02	1.5261152937E-01
Al3	H15	1.3514279699E+01	2.2230777162E-03	8.3070679725E-03	1.1004565846E-01
Al4	H15	1.3509145918E+01	1.2026780100E-02	4.4941746089E-02	5.9534353009E-01
C5	H15	6.0648901130E+00	1.0180112744E-02	8.4700711063E-02	5.0393074517E-01
C6	H15	6.0671475584E+00	5.7517413642E-03	4.7855374853E-02	2.8471976536E-01
C7	H15	6.0633851528E+00	1.0189985925E-02	8.4803814897E-02	5.0441948235E-01
C8	H15	6.0451284354E+00	4.9702300194E-02	4.1353378678E-01	2.4603378964E+00
C9	H15	5.5885687622E+00	9.6291020605E-01	8.0115607834E+00	4.7665489556E+01 (Bonded)
C10	H15	6.0436979565E+00	4.9571094663E-02	4.1254380926E-01	2.4538430272E+00
H11	H15	1.0191977822E+00	1.8847594548E-03	9.3307773328E-02	9.3298400562E-02
H12	H15	1.0200257610E+00	4.3119568320E-04	2.1344855544E-02	2.1344828630E-02
H13	H15	1.0184746059E+00	1.8753744642E-03	9.2909446422E-02	9.2833829546E-02
H14	H15	1.0167906447E+00	6.6976097384E-03	3.3157519708E-01	3.3154165885E-01
Al1	H16	1.3502617502E+01	3.0950480045E-03	1.1565591264E-02	1.5333426326E-01
Al2	H16	1.3502825346E+01	3.1311911718E-03	1.1700455496E-02	1.5512486100E-01
Al3	H16	1.3500834113E+01	7.1177950442E-03	2.6597364013E-02	3.5262841080E-01
Al4	H16	1.3500682956E+01	6.9566269017E-03	2.5995566333E-02	3.4464385019E-01
C5	H16	6.0402579364E+00	4.9565503002E-02	4.1239556517E-01	2.4555644614E+00
C6	H16	6.0599950857E+00	1.0177653334E-02	8.4679644752E-02	5.0421931210E-01
C7	H16	6.0607267487E+00	5.6302725826E-03	4.6856649012E-02	2.7893386377E-01
C8	H16	6.0599495364E+00	1.0181136330E-02	8.4709235663E-02	5.0439186599E-01
C9	H16	6.0403091118E+00	4.9550472791E-02	4.1226754282E-01	2.4548198376E+00
C10	H16	5.5818868801E+00	9.6331672041E-01	8.0169774759E+00	4.7724448669E+01 (Bonded)
H11	H16	1.0159822455E+00	6.6555427724E-03	3.2949237888E-01	3.2972759911E-01
H12	H16	1.0184734456E+00	1.8753718624E-03	9.2833817806E-02	9.2909306236E-02

H13	H16	1.0183707893E+00	4.2390234199E-04	2.1000889520E-02	2.1000886969E-02
H14	H16	1.0183717666E+00	1.8750772200E-03	9.2828504948E-02	9.2894709120E-02
H15	H16	1.0160797423E+00	6.6653491594E-03	3.2994471213E-01	3.3021342521E-01
Al1	K17	2.4558763158E+02	1.7962944585E-01	6.7124023498E-01	4.8916097165E-01
Al2	K17	2.4559167920E+02	1.7975427505E-01	6.7169546029E-01	4.8950090238E-01
Al3	K17	2.4559171696E+02	1.7975399343E-01	6.7169430509E-01	4.8950013549E-01 (Bonded)
Al4	K17	2.4558756344E+02	1.7962905035E-01	6.7123894378E-01	4.8915989462E-01
C5	K17	1.1033785622E+02	3.4195253395E-03	2.8451180753E-02	9.3119384168E-03
C6	K17	1.1033864146E+02	3.4218026022E-03	2.8469925164E-02	9.3181397834E-03
C7	K17	1.1031058118E+02	3.4350253369E-03	2.8587208558E-02	9.3541474975E-03
C8	K17	1.1033784564E+02	3.4194712312E-03	2.8450733296E-02	9.3117910709E-03
C9	K17	1.1033864938E+02	3.4218199394E-03	2.8470067367E-02	9.3181869954E-03
C10	K17	1.1031064218E+02	3.4351066510E-03	2.8587869456E-02	9.3543689295E-03
H11	K17	1.8543740959E+01	5.5447357127E-04	2.7450025080E-02	1.5099241084E-03
H12	K17	1.8545579870E+01	5.5575082846E-04	2.7510528546E-02	1.5134022930E-03
H13	K17	1.8530516586E+01	5.4094917523E-04	2.6799601558E-02	1.4730949200E-03
H14	K17	1.8543728013E+01	5.5446926374E-04	2.7449830996E-02	1.5099123783E-03
H15	K17	1.8545603243E+01	5.5577390322E-04	2.7511636093E-02	1.5134651294E-03
H16	K17	1.8530518834E+01	5.4095530953E-04	2.6799902207E-02	1.4731116247E-03

Benzene-MgAl$_4$ π-π

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7208978533E+02	7.7002872327E-01	2.9317116752E+00	2.9316151242E+00 (Bonded)
Al1	Al3	1.7209051050E+02	7.6858999585E-01	2.9262340432E+00	2.9261375742E+00 (Bonded)
Al2	Al3	1.7222164100E+02	5.1768968975E-01	1.9709224841E+00	1.9709224178E+00
Al1	Al4	1.7221083308E+02	5.1664790223E-01	1.9670210229E+00	1.9670205952E+00
Al2	Al4	1.7209054211E+02	7.6859017223E-01	2.9261383441E+00	2.9262340783E+00 (Bonded)
Al3	Al4	1.7208982810E+02	7.7002980951E-01	2.9316191611E+00	2.9317151732E+00 (Bonded)
Al1	C5	7.9348481986E+01	4.2557882001E-02	1.6202959158E-01	3.5208750373E-01
Al2	C5	7.9354994497E+01	3.4760850633E-02	1.3233978470E-01	2.8758153723E-01
Al3	C5	7.9313922440E+01	1.1691030585E-01	4.4509509700E-01	9.6721584373E-01 (Bonded)
Al4	C5	7.9356279631E+01	2.6997113185E-02	1.0278543165E-01	2.2335101612E-01
Al1	C6	7.9289197055E+01	1.1553193531E-01	4.3986193420E-01	9.5608700844E-01 (Bonded)
Al2	C6	7.9336025199E+01	2.7102134518E-02	1.0318190095E-01	2.2428429545E-01
Al3	C6	7.9327378859E+01	4.4400154341E-02	1.6903805751E-01	3.6743442948E-01
Al4	C6	7.9329609680E+01	3.4741197054E-02	1.3226928787E-01	2.8750152131E-01
C5	C6	3.5840850799E+01	1.3487574513E+00	1.1158465174E+01	1.1161671215E+01 (Bonded)
Al1	C7	7.9211419004E+01	8.3817135032E-02	3.1911494458E-01	6.9445000237E-01
Al2	C7	7.9214653521E+01	8.2568423104E-02	3.1435040102E-01	6.8410405102E-01
Al3	C7	7.9240101243E+01	3.1678311280E-02	1.2060408986E-01	2.6246427220E-01
Al4	C7	7.9237344042E+01	3.2001529884E-02	1.2183862179E-01	2.6514223488E-01
C5	C7	3.6438644206E+01	6.6989141464E-02	5.5421084147E-01	5.5502504865E-01
C6	C7	3.5792338704E+01	1.3386478751E+00	1.1078009200E+01	1.1091097539E+01 (Bonded)
Al1	C8	7.9354026042E+01	2.6993199955E-02	1.0277055526E-01	2.2332493934E-01
Al2	C8	7.9311695664E+01	1.1688179927E-01	4.4498658315E-01	9.6700727502E-01 (Bonded)
Al3	C8	7.9352762384E+01	3.4753699421E-02	1.3231255451E-01	2.8753048279E-01
Al4	C8	7.9346265115E+01	4.2549573405E-02	1.6199792323E-01	3.5202869298E-01
C5	C8	3.6486926301E+01	7.5529394091E-02	6.2486558479E-01	6.2488320695E-01
C6	C8	3.6480694234E+01	6.7011067479E-02	5.5455152609E-01	5.5440787327E-01
C7	C8	3.5801628198E+01	1.3389640743E+00	1.1093717343E+01	1.1077755552E+01 (Bonded)
Al1	C9	7.9329582125E+01	3.4741086258E-02	1.3226889480E-01	2.8750064192E-01
Al2	C9	7.9327365961E+01	4.4399902523E-02	1.6903710448E-01	3.6743239350E-01
Al3	C9	7.9336017895E+01	2.7101373628E-02	1.0317900066E-01	2.2427802796E-01
Al4	C9	7.9289204532E+01	1.1553078406E-01	4.3985745543E-01	9.5607760602E-01 (Bonded)
C5	C9	3.6481716908E+01	6.7015703849E-02	5.5443059592E-01	5.5458996683E-01
C6	C9	3.6467150713E+01	7.5171071346E-02	6.2207981309E-01	6.2207989427E-01
C7	C9	3.6428139515E+01	6.7036737587E-02	5.5541939674E-01	5.5476403200E-01
C8	C9	3.5839831977E+01	1.3487260532E+00	1.1158520091E+01	1.1161412835E+01 (Bonded)
Al1	C10	7.9237244541E+01	3.2000830655E-02	1.2183598613E-01	2.6513671794E-01
Al2	C10	7.9240016222E+01	3.1677783695E-02	1.2060208532E-01	2.6246017459E-01
Al3	C10	7.9214574536E+01	8.2566487155E-02	3.1434301999E-01	6.8408872421E-01
Al4	C10	7.9211354475E+01	8.3815432513E-02	3.1910839323E-01	6.9443662039E-01
C5	C10	3.5802608068E+01	1.3389853788E+00	1.1077619407E+01	1.1093905422E+01 (Bonded)

C6	C10	3.6428106368E+01	6.7036529628E-02	5.5476223865E-01	5.5541825272E-01	
C7	C10	3.6383862632E+01	6.9469021547E-02	5.7557159594E-01	5.7557219593E-01	
C8	C10	3.6437579017E+01	6.6986400311E-02	5.5420379247E-01	5.5500291592E-01	
C9	C10	3.5792296746E+01	1.3386462584E+00	1.1077997267E+01	1.1091095705E+01	(Bonded)
Al1	H11	1.2905377060E+01	3.9951187136E-03	1.5210518546E-02	2.0324386784E-01	
Al2	H11	1.2904692525E+01	6.2143806541E-03	2.3659081490E-02	3.1614448804E-01	
Al3	H11	1.2896095876E+01	2.3408548074E-02	8.9119859022E-02	1.1908642001E+00	
Al4	H11	1.2906138531E+01	2.4777896791E-03	9.4336264759E-03	1.2605271437E-01	
C5	H11	5.4628917671E+00	9.5408505352E-01	7.8932834306E+00	4.8537215144E+01	(Bonded)
C6	H11	5.9150859047E+00	4.6284444518E-02	3.8302791326E-01	2.3546307880E+00	
C7	H11	5.9262626658E+00	9.9158006890E-03	8.2155370849E-02	5.0444700877E-01	
C8	H11	5.9378837758E+00	3.7660151457E-03	3.1157665833E-02	1.9158867093E-01	
C9	H11	5.9333262189E+00	9.8022664067E-03	8.1118876460E-02	4.9867117373E-01	
C10	H11	5.9082296682E+00	4.5969430233E-02	3.8087085892E-01	2.3386050510E+00	
Al1	H12	1.2897749829E+01	2.2947038167E-02	8.7365701657E-02	1.1672186030E+00	
Al2	H12	1.2908392148E+01	2.5127134644E-03	9.5662779483E-03	1.2781108735E-01	
Al3	H12	1.2907550898E+01	4.1960833511E-03	1.5975119666E-02	2.1343698091E-01	
Al4	H12	1.2906164930E+01	6.1224497803E-03	2.3309849433E-02	3.1142307898E-01	
C5	H12	5.9176195905E+00	4.6330965227E-02	3.8330276614E-01	2.3566598929E+00	
C6	H12	5.4623598219E+00	9.5343767989E-01	7.8901939680E+00	4.8497334980E+01	(Bonded)
C7	H12	5.9090873640E+00	4.5965466705E-02	3.8083762288E-01	2.3380685317E+00	
C8	H12	5.9357136337E+00	9.8078099895E-03	8.1143716736E-02	4.9888173764E-01	
C9	H12	5.9372013629E+00	3.7530481235E-03	3.1058434289E-02	1.9090165606E-01	
C10	H12	5.9270946085E+00	9.9386102722E-03	8.2344440897E-02	5.0553499381E-01	
H11	H12	9.6307760299E-01	6.0652662409E-03	3.0855858327E-01	3.0851439463E-01	
Al1	H13	1.2855568655E+01	1.2154365819E-02	4.6275022085E-02	6.2052807361E-01	
Al2	H13	1.2856213764E+01	1.1711328397E-02	4.4586788021E-02	5.9790927460E-01	
Al3	H13	1.2859876400E+01	4.3869210260E-03	1.6701667363E-02	2.2396953440E-01	
Al4	H13	1.2859405988E+01	4.4852940264E-03	1.7076747408E-02	2.2899186213E-01	
C5	H13	5.9139782650E+00	9.8235671975E-03	8.1271790081E-02	5.0153165702E-01	
C6	H13	5.8943153918E+00	4.5749069160E-02	3.7859740300E-01	2.3356695182E+00	
C7	H13	5.4328054034E+00	9.5480357780E-01	7.9108328699E+00	4.8746469676E+01	(Bonded)
C8	H13	5.8958423848E+00	4.5761493414E-02	3.7860212045E-01	2.3363038251E+00	
C9	H13	5.9122716053E+00	9.8350979913E-03	8.1390574978E-02	5.0212034929E-01	
C10	H13	5.9085277821E+00	3.3464984712E-03	2.7726768434E-02	1.7085187995E-01	
H11	H13	9.6165938823E-01	1.7804122694E-03	9.0574999623E-02	9.0897033398E-02	
H12	H13	9.5970952738E-01	5.9558667384E-03	3.0294970547E-01	3.0407037019E-01	
Al1	H14	1.2906207631E+01	2.4778051313E-03	9.4336873585E-03	1.2605279815E-01	
Al2	H14	1.2896167171E+01	2.3408923078E-02	8.9121289716E-02	1.1908766425E+00	
Al3	H14	1.2904764835E+01	6.2144631847E-03	2.3659394900E-02	3.1614692517E-01	
Al4	H14	1.2905451776E+01	3.9951289302E-03	1.5210554136E-02	2.0324325519E-01	
C5	H14	5.9380842364E+00	3.7663049936E-03	3.1159185118E-02	1.9160234885E-01	
C6	H14	5.9333600508E+00	9.8023233996E-03	8.1119337521E-02	4.9867129473E-01	
C7	H14	5.9082685608E+00	4.5970103767E-02	3.8087604232E-01	2.3386262858E+00	
C8	H14	5.4627963592E+00	9.5400703640E-01	7.8928605681E+00	4.8532975768E+01	(Bonded)
C9	H14	5.9151179662E+00	4.6284942804E-02	3.8303208681E-01	2.3546430181E+00	
C10	H14	5.9262895054E+00	9.9158487692E-03	8.2155854848E-02	5.0444664417E-01	
H11	H14	9.6583432933E-01	2.8586449382E-04	1.4542798241E-02	1.4542717215E-02	
H12	H14	9.6520804333E-01	1.8151511596E-03	9.2329048537E-02	9.2341758373E-02	
H13	H14	9.5958362987E-01	5.9426549128E-03	3.0339585464E-01	3.0231928683E-01	
Al1	H15	1.2906152608E+01	6.1226939182E-03	2.3310784002E-02	3.1143572384E-01	
Al2	H15	1.2907540942E+01	4.1963405503E-03	1.5976099400E-02	2.1345021885E-01	
Al3	H15	1.2908383124E+01	2.5128447965E-03	9.5667776278E-03	1.2781786066E-01	
Al4	H15	1.2897742847E+01	2.2947831188E-02	8.7368701907E-02	1.1672597899E+00	
C5	H15	5.9358765850E+00	9.8083313634E-03	8.1145741825E-02	4.9890862072E-01	
C6	H15	5.9371977988E+00	3.7530838594E-03	3.1058725969E-02	1.9090361269E-01	
C7	H15	5.9270964708E+00	9.9386210972E-03	8.2344444747E-02	5.0553591225E-01	
C8	H15	5.9174515661E+00	4.6323300413E-02	3.8325016197E-01	2.3562717307E+00	
C9	H15	5.4623551223E+00	9.5343688687E-01	7.8901884349E+00	4.8497329928E+01	(Bonded)
C10	H15	5.9090770378E+00	4.5965119596E-02	3.8083514397E-01	2.3380525769E+00	
H11	H15	9.6520196563E-01	1.8151351200E-03	9.2341456886E-02	9.2328299851E-02	
H12	H15	9.6610549125E-01	2.8483642339E-04	1.4488421982E-02	1.4488432524E-02	
H13	H15	9.6179411969E-01	1.7852812580E-03	9.1145614373E-02	9.0809759276E-02	
H14	H15	9.6308226848E-01	6.0652949951E-03	3.0855832692E-01	3.0851608170E-01	
Al1	H16	1.2859410354E+01	4.4853231495E-03	1.7076862001E-02	2.2899322117E-01	
Al2	H16	1.2859883147E+01	4.3869186470E-03	1.6701658868E-02	2.2396928794E-01	

Al3	H16	1.2856221397E+01	1.1711283790E-02	4.4586616693E-02	5.9790666350E-01
Al4	H16	1.2855578559E+01	1.2154506998E-02	4.6275549530E-02	6.2053493503E-01
C5	H16	5.8960094388E+00	4.5767826614E-02	3.7864383907E-01	2.3366258557E+00
C6	H16	5.9122756734E+00	9.8351110271E-03	8.1390672235E-02	5.0212073458E-01
C7	H16	5.9085372365E+00	3.3465087499E-03	2.7726824693E-02	1.7085230936E-01
C8	H16	5.9138146978E+00	9.8234743180E-03	8.1273313643E-02	5.0152663524E-01
C9	H16	5.8943177716E+00	4.5749370380E-02	3.7859994516E-01	2.3356835930E+00
C10	H16	5.4328024501E+00	9.5480375970E-01	7.9108426234E+00	4.8746451756E+01 (Bonded)
H11	H16	9.5957883028E-01	5.9426026149E-03	3.0231831069E-01	3.0339301530E-01
H12	H16	9.6179535581E-01	1.7852844849E-03	9.0809857344E-02	9.1145728250E-02
H13	H16	9.5900896471E-01	2.6200880215E-04	1.3376577576E-02	1.3376570111E-02
H14	H16	9.6166528615E-01	1.7804167878E-03	9.0574724843E-02	9.0897213351E-02
H15	H16	9.5970938425E-01	5.9558267270E-03	3.0294789068E-01	3.0406815774E-01
Al1	Mg17	1.4873574918E+02	3.5314558858E-01	1.3445226312E+00	1.5572158926E+00
Al2	Mg17	1.4874105552E+02	3.5234158460E-01	1.3414173876E+00	1.5536705906E+00 (Bonded)
Al3	Mg17	1.4874106111E+02	3.5234041546E-01	1.3414128913E+00	1.5536654351E+00
Al4	Mg17	1.4873578139E+02	3.5314593572E-01	1.3445236604E+00	1.5572174233E+00
C5	Mg17	6.8521743909E+01	1.4501770879E-02	1.1997524473E-01	6.3946397219E-02
C6	Mg17	6.8502076486E+01	1.4468538303E-02	1.1973469903E-01	6.3799856253E-02
C7	Mg17	6.8421254179E+01	1.4420758585E-02	1.1948029278E-01	6.3589168824E-02
C8	Mg17	6.8519811770E+01	1.4500913011E-02	1.1997153075E-01	6.3942614398E-02
C9	Mg17	6.8502067693E+01	1.4468244049E-02	1.1973227955E-01	6.3798558724E-02
C10	Mg17	6.8421183160E+01	1.4420133330E-02	1.1947523690E-01	6.3586411727E-02
H11	Mg17	1.1143982905E+01	8.6050755023E-04	4.3776642286E-02	3.7944577994E-03
H12	Mg17	1.1145580576E+01	8.5760414120E-04	4.3622688921E-02	3.7816550494E-03
H13	Mg17	1.1104530091E+01	8.0035753475E-04	4.0861393071E-02	3.5292228281E-03
H14	Mg17	1.1144044992E+01	8.6051839527E-04	4.3776950097E-02	3.7945056212E-03
H15	Mg17	1.1145572451E+01	8.5763469710E-04	4.3624274911E-02	3.7817897874E-03
H16	Mg17	1.1104536288E+01	8.0036053820E-04	4.0861523603E-02	3.5292360720E-03

Benzene-CaAl₄ π-π

Atom A	Atom B	2*D2(A,B)	DI(A,B)	%Deloc(A,B)	%Deloc(B,A)
Al1	Al2	1.7384783809E+02	8.2119772887E-01	3.1105190497E+00	3.1103467511E+00 (Bonded)
Al1	Al3	1.7384799845E+02	8.2093690558E-01	3.1095311076E+00	3.1093583294E+00 (Bonded)
Al2	Al3	1.7399859770E+02	5.3904460949E-01	2.0416710749E+00	2.0416707241E+00
Al1	Al4	1.7397918476E+02	5.3918892974E-01	2.0423308277E+00	2.0423308883E+00
Al2	Al4	1.7384796480E+02	8.2093398821E-01	3.1093478139E+00	3.1095201494E+00 (Bonded)
Al3	Al4	1.7384786276E+02	8.2119794433E-01	3.1103470327E+00	3.1105199580E+00 (Bonded)
Al1	C5	7.9472010362E+01	2.9661476873E-02	1.1235124698E-01	2.4629319696E-01
Al2	C5	7.9479970010E+01	2.2548577229E-02	8.5404393435E-02	1.8723144489E-01
Al3	C5	7.9456484298E+01	6.9547320149E-02	2.6341554110E-01	5.7748411830E-01 (Bonded)
Al4	C5	7.9478540274E+01	1.6596941269E-02	6.2865618961E-02	1.3781221152E-01
Al1	C6	7.9466588979E+01	7.4235100237E-02	2.8118647352E-01	6.1627820056E-01 (Bonded)
Al2	C6	7.9499572658E+01	1.7076008997E-02	6.4676639057E-02	1.4176005776E-01
Al3	C6	7.9496183415E+01	2.3881818633E-02	9.0454127697E-02	1.9825990894E-01
Al4	C6	7.9492135296E+01	2.3137754489E-02	8.7640802827E-02	1.9208290493E-01
C5	C6	3.5585799970E+01	1.3626046459E+00	1.1314347423E+01	1.1311947267E+01 (Bonded)
Al1	C7	7.9417728850E+01	4.6241773032E-02	1.7515381601E-01	3.8418948969E-01
Al2	C7	7.9418348112E+01	5.3804550893E-02	2.0378869081E-01	4.4702314800E-01
Al3	C7	7.9435228521E+01	2.0071036001E-02	7.6020510890E-02	1.6675573996E-01
Al4	C7	7.9431534640E+01	1.8625485271E-02	7.0549304296E-02	1.5474570312E-01
C5	C7	3.6203223486E+01	7.0411011142E-02	5.8465575095E-01	5.8499423065E-01
C6	C7	3.5565452100E+01	1.3613318403E+00	1.1301380805E+01	1.1310322912E+01 (Bonded)
Al1	C8	7.9478554289E+01	1.6596384904E-02	6.2863509708E-02	1.3780757203E-01
Al2	C8	7.9456481870E+01	6.9547621837E-02	2.6341672903E-01	5.7748654067E-01 (Bonded)
Al3	C8	7.9479995082E+01	2.2548516188E-02	8.5404147563E-02	1.8723091123E-01
Al4	C8	7.9472019548E+01	2.9661156181E-02	1.1235003560E-01	2.4629049884E-01
C5	C8	3.6215680800E+01	8.7466407223E-02	7.2627472846E-01	7.2627462446E-01
C6	C8	3.6231833615E+01	7.0547741420E-02	5.8566682064E-01	5.8579100289E-01
C7	C8	3.5558203261E+01	1.3604618390E+00	1.1303094700E+01	1.1296553072E+01 (Bonded)
Al1	C9	7.9492108322E+01	2.3137689824E-02	8.7640555295E-02	1.9208243905E-01
Al2	C9	7.9496140512E+01	2.3881571178E-02	9.0453205985E-02	1.9825792786E-01
Al3	C9	7.9499557121E+01	1.7075678087E-02	6.4675374597E-02	1.4175736299E-01

Al4	C9	7.9466557561E+01	7.4234499551E-02	2.8118420658E-01	6.1627344144E-01 (Bonded)
C5	C9	3.6231814906E+01	7.0547984080E-02	5.8579310169E-01	5.8566905144E-01
C6	C9	3.6230633411E+01	8.8301194762E-02	7.3305082422E-01	7.3305109496E-01
C7	C9	3.6210884729E+01	7.0439810881E-02	5.8523350688E-01	5.8477102868E-01
C8	C9	3.5585791700E+01	1.3626047831E+00	1.1314346942E+01	1.1311952584E+01 (Bonded)
Al1	C10	7.9431558240E+01	1.8625546564E-02	7.0549534373E-02	1.5474617092E-01
Al2	C10	7.9435236046E+01	2.0071238965E-02	7.6021292691E-02	1.6675738157E-01
Al3	C10	7.9418383395E+01	5.3803842598E-02	2.0378597307E-01	4.4701714357E-01
Al4	C10	7.9417747390E+01	4.6242536435E-02	1.7515671280E-01	3.8419572935E-01
C5	C10	3.5558207713E+01	1.3604619671E+00	1.1296555753E+01	1.1303092737E+01 (Bonded)
C6	C10	3.6210907788E+01	7.0439880052E-02	5.8477138695E-01	5.8523392483E-01
C7	C10	3.6174839734E+01	8.5262552296E-02	7.0838495819E-01	7.0838476847E-01
C8	C10	3.6203238312E+01	7.0411147767E-02	5.8465680170E-01	5.8499520909E-01
C9	C10	3.5565448439E+01	1.3613318050E+00	1.1301384686E+01	1.1310319589E+01 (Bonded)
Al1	H11	1.3038483399E+01	3.4214601138E-03	1.2959749507E-02	1.7317384812E-01
Al2	H11	1.3039015498E+01	3.8019928183E-03	1.4400327222E-02	1.9243413776E-01
Al3	H11	1.3033435274E+01	1.4966923371E-02	5.6688312503E-02	7.5753614787E-01
Al4	H11	1.3039265800E+01	1.8558846864E-03	7.0296892446E-03	9.3933783278E-02
C5	H11	5.4701100285E+00	9.5683669758E-01	7.9450652517E+00	4.8429351048E+01 (Bonded)
C6	H11	5.9260460469E+00	4.7488964950E-02	3.9423956824E-01	2.4036073870E+00
C7	H11	5.9401151713E+00	9.9427333816E-03	8.2606989600E-02	5.0324169895E-01
C8	H11	5.9461112485E+00	4.8359610503E-03	4.0155253968E-02	2.4476742578E-01
C9	H11	5.9448302384E+00	9.9161870432E-03	8.2321329733E-02	5.0189808207E-01
C10	H11	5.9213901321E+00	4.7395996180E-02	3.9377899061E-01	2.3989018638E+00
Al1	H12	1.3047613940E+01	1.6702366760E-02	6.3264946011E-02	8.4435274088E-01
Al2	H12	1.3055788325E+01	1.8000758838E-03	6.8179197046E-03	9.0999019971E-02
Al3	H12	1.3055401412E+01	2.5783885664E-03	9.7658345129E-03	1.3034496754E-01
Al4	H12	1.3053937253E+01	4.0549664402E-03	1.5359334651E-02	2.0499023146E-01
C5	H12	5.9319644272E+00	4.7516368239E-02	3.9455075996E-01	2.4020892570E+00
C6	H12	5.4786795953E+00	9.5661338910E-01	7.9415259922E+00	4.8359561772E+01 (Bonded)
C7	H12	5.9285258002E+00	4.7501618518E-02	3.9465663578E-01	2.4013436161E+00
C8	H12	5.9507517127E+00	9.9435027374E-03	8.2565569408E-02	5.0267269969E-01
C9	H12	5.9545296959E+00	4.9087876990E-03	4.0751342124E-02	2.4815335501E-01
C10	H12	5.9473016289E+00	9.9531493401E-03	8.2693506128E-02	5.0316036324E-01
H11	H12	9.7392175426E-01	6.2857021374E-03	3.1814464909E-01	3.1776034525E-01
Al1	H13	1.3013898514E+01	7.0258137125E-03	2.6612259903E-02	3.5622703992E-01
Al2	H13	1.3013467362E+01	9.3303253075E-03	3.5339292824E-02	4.7307177528E-01
Al3	H13	1.3016650126E+01	2.9692705946E-03	1.1246328667E-02	1.5054974668E-01
Al4	H13	1.3016130507E+01	2.5610570387E-03	9.7007293887E-03	1.2985225702E-01
C5	H13	5.9331696482E+00	9.9319419167E-03	8.2469586297E-02	5.0357530307E-01
C6	H13	5.9157143559E+00	4.7362420475E-02	3.9318903283E-01	2.4013979789E+00
C7	H13	5.4560312382E+00	9.5733710990E-01	7.9538225201E+00	4.8539482944E+01 (Bonded)
C8	H13	5.9144554367E+00	4.7362065401E-02	3.9326945458E-01	2.4013799757E+00
C9	H13	5.9344350949E+00	9.9165551410E-03	8.2324385575E-02	5.0279515351E-01
C10	H13	5.9323711677E+00	4.6604298534E-03	3.8720134851E-02	2.3629592234E-01
H11	H13	9.7328364140E-01	1.7914685367E-03	9.0673423032E-02	9.0832117109E-02
H12	H13	9.7221628790E-01	6.2825480601E-03	3.1760089756E-01	3.1854153699E-01
Al1	H14	1.3039277688E+01	1.8559130478E-03	7.0297964628E-03	9.3935135803E-02
Al2	H14	1.3033444415E+01	1.4967192114E-02	5.6689340128E-02	7.5754908103E-01
Al3	H14	1.3039029214E+01	3.8020757260E-03	1.4400638767E-02	1.9243816411E-01
Al4	H14	1.3038494534E+01	3.4214482750E-03	1.2959705048E-02	1.7317309598E-01
C5	H14	5.9461156504E+00	4.8359601359E-03	4.0155252126E-02	2.4476716334E-01
C6	H14	5.9448376941E+00	9.9161791552E-03	8.2321233846E-02	5.0189723959E-01
C7	H14	5.9213936885E+00	4.7396199283E-02	3.9378078352E-01	2.3989100252E+00
C8	H14	5.4701152426E+00	9.5683847916E-01	7.9450789073E+00	4.8429398451E+01 (Bonded)
C9	H14	5.9260490769E+00	4.7489018782E-02	3.9424016075E-01	2.4036079890E+00
C10	H14	5.9401219927E+00	9.9427754047E-03	8.2607316616E-02	5.0324338149E-01
H11	H14	9.7571660515E-01	3.3722741320E-04	1.7068434789E-02	1.7068419716E-02
H12	H14	9.7616187434E-01	1.8071877074E-03	9.1358543134E-02	9.1468952666E-02
H13	H14	9.7104959729E-01	6.2612773663E-03	3.1746305746E-01	3.1690813339E-01
Al1	H15	1.3054002860E+01	4.0549622450E-03	1.5359318305E-02	2.0498899541E-01
Al2	H15	1.3055464351E+01	2.5784651504E-03	9.7661262584E-03	1.3034818796E-01
Al3	H15	1.3055855800E+01	1.8000558799E-03	6.8178427665E-03	9.0997554159E-02
Al4	H15	1.3047678754E+01	1.6702400853E-02	6.3265077025E-02	8.4435024669E-01
C5	H15	5.9507805854E+00	9.9435522468E-03	8.2565992330E-02	5.0267269157E-01
C6	H15	5.9545616507E+00	4.9087914417E-03	4.0751358144E-02	2.4815230464E-01

C7	H15	5.9473297666E+00	9.9531515706E-03	8.2693546807E-02	5.0315796260E-01
C8	H15	5.9319947002E+00	4.7517028269E-02	3.9455618400E-01	2.4021106243E+00
C9	H15	5.4787048772E+00	9.5661793817E-01	7.9415666903E+00	4.8359550173E+01 (Bonded)
C10	H15	5.9285569398E+00	4.7501993663E-02	3.9465964690E-01	2.4013505855E+00
H11	H15	9.7616588630E-01	1.8071993894E-03	9.1469624713E-02	9.1358677332E-02
H12	H15	9.7808006839E-01	3.4219842553E-04	1.7299115909E-02	1.7299029496E-02
H13	H15	9.7446309905E-01	1.7986700439E-03	9.1197252268E-02	9.0927496508E-02
H14	H15	9.7392746810E-01	6.2857615259E-03	3.1814737402E-01	3.1776176022E-01
Al1	H16	1.3016077536E+01	2.5610648628E-03	9.7007587370E-03	1.2985318593E-01
Al2	H16	1.3016594553E+01	2.9692308928E-03	1.1246180227E-02	1.5054835073E-01
Al3	H16	1.3013416423E+01	9.3299652682E-03	3.5337923076E-02	4.7305545921E-01
Al4	H16	1.3013844753E+01	7.0258587498E-03	2.6612431283E-02	3.5623078347E-01
C5	H16	5.9144305200E+00	4.7361522272E-02	3.9326500104E-01	2.4013622799E+00
C6	H16	5.9344129507E+00	9.9165444042E-03	8.2324266037E-02	5.0279666988E-01
C7	H16	5.9323452609E+00	4.6604165709E-03	3.8720034867E-02	2.3629621737E-01
C8	H16	5.9331461835E+00	9.9318958010E-03	8.2469191569E-02	5.0357502884E-01
C9	H16	5.9156879451E+00	4.7362168404E-02	3.9318708543E-01	2.4013950406E+00
C10	H16	5.4560102897E+00	9.5733353794E-01	7.9537907130E+00	4.8539500780E+01 (Bonded)
H11	H16	9.7104477598E-01	6.2612138400E-03	3.1690519793E-01	3.1746113765E-01
H12	H16	9.7445423332E-01	1.7986620378E-03	9.0927545981E-02	9.1197220118E-02
H13	H16	9.7230915034E-01	3.2847392377E-04	1.6654482789E-02	1.6654551050E-02
H14	H16	9.7328051160E-01	1.7914632103E-03	9.0673073371E-02	9.0832219336E-02
H15	H16	9.7221714970E-01	6.2825735015E-03	3.1760059721E-01	3.1854413252E-01
Al1	Ca17	2.5252397119E+02	4.2198301858E-01	1.5983802339E+00	1.1020074539E+00 (Bonded)
Al2	Ca17	2.5253756317E+02	4.2279971716E-01	1.6013850019E+00	1.1041402599E+00
Al3	Ca17	2.5253760641E+02	4.2280010969E-01	1.6013862135E+00	1.1041412850E+00
Al4	Ca17	2.5252396433E+02	4.2198174552E-01	1.5983754592E+00	1.1020041293E+00
C5	Ca17	1.1528395861E+02	1.1640512808E-02	9.6656654216E-02	3.0399166118E-02
C6	Ca17	1.1530846702E+02	1.1547818603E-02	9.5866629748E-02	3.0157095465E-02
C7	Ca17	1.1521714465E+02	1.1854297299E-02	9.8488793387E-02	3.0957463711E-02
C8	Ca17	1.1528397526E+02	1.1640238038E-02	9.6654358832E-02	3.0398448557E-02
C9	Ca17	1.1530842453E+02	1.1547606009E-02	9.5864900265E-02	3.0156540278E-02
C10	Ca17	1.1521717549E+02	1.1854344308E-02	9.8489157567E-02	3.0957586473E-02
H11	Ca17	1.8913235892E+01	1.2007398706E-03	6.0774270948E-02	3.1357287600E-03
H12	Ca17	1.8936105174E+01	1.2114954996E-03	6.1244586494E-02	3.1638170546E-03
H13	Ca17	1.8880207005E+01	1.1692509600E-03	5.9284066651E-02	3.0534955595E-03
H14	Ca17	1.8913252585E+01	1.2007601888E-03	6.0775245661E-02	3.1357818209E-03
H15	Ca17	1.8936199763E+01	1.2115047292E-03	6.1244747146E-02	3.1638411576E-03
H16	Ca17	1.8880129624E+01	1.1692437055E-03	5.9283941811E-02	3.0534766144E-03