

Supporting Information

Adsorption of Gases on B₁₂N₁₂ and Al₁₂N₁₂ Nanocages

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Table S1. Change in structural parameters due to gas adsorption on B₁₂N₁₂.

gas	bond angle of gas		bond length of gas		bond angle of cage	
	gas/B ₁₂ N ₁₂	gas	gas/B ₁₂ N ₁₂	gas	gas/B ₁₂ N ₁₂	cage
SiH ₄	109	109	1.48	1.48	125	125
H ₂	-	-	0.74	0.74	125	125
Cl ₂	-	-	2.02	2.02	125	125
F ₂	-	-	1.37	1.37	125	125
CF ₄	109	109	1.33	1.32	125	125
CH ₄	109	109	1.09	1.09	125	125
CF ₂ Cl ₂	109	109	1.76	1.76	125	125
N ₂	-	-	1.09	1.09	125	125
CHF ₃	110	110	1.33	1.33	125	125
OCS	179	180	1.15	1.15	125	125
N ₂ O	179	180	1.18	1.18	125	125
AsH ₃	99	92	1.51	1.52	119	125
CH ₃ Cl	107	108	1.09	1.09	124	125
COCl ₂	123	123	1.18	1.17	124	125
C ₂ H ₂	179	179	1.19	1.19	125	125
C ₂ H ₄	116	116	1.33	1.32	124	125
H ₂ Se	91	91	1.47	1.47	121	125

H ₂ S	93	92	1.34	1.34	120	125
PH ₃	101	93	1.40	1.41	118	125
COF ₂	125	126	1.17	1.17	124	125
CH ₃ F	107	109	1.09	1.09	123	125
HCHO	119	121	1.22	1.20	118	125
(CH ₃) ₂ O	112	111	1.44	1.40	117	125
CH ₃ NH ₂	107	115	1.48	1.46	116	125

Table S2. Change in structural parameters due to gas adsorption on Al₁₂N₁₂.

gas	bond angle of gas		bond length of gas		bond angle of cage	
	gas/Al ₁₂ N ₁₂	gas	gas/Al ₁₂ N ₁₂	gas	gas/Al ₁₂ N ₁₂	cage
SiH ₄	108	109	1.51	1.48	123	125
H ₂	-	-	0.75	0.74	124	125
Cl ₂	-	-	2.12	2.02	122	125
F ₂	-	-	1.38	1.37	125	125
CF ₄	108	109	1.30	1.32	124	125
CH ₄	111	109	1.09	1.09	124	125
CF ₂ Cl ₂	110	109	1.74	1.76	124	125
N ₂	-	-	1.09	1.09	123	125
CHF ₃	112	110	1.41	1.33	123	125
OCS	178	180	1.16	1.15	122	125
N ₂ O	178	180	1.20	1.18	122	125
AsH ₃	98	92	1.51	1.52	121	125
CH ₃ Cl	106	108	1.09	1.09	122	125
COCl ₂	123	123	1.19	1.17	122	125
C ₂ H ₂	178	179	1.20	1.19	122	125
C ₂ H ₄	117	116	1.34	1.32	121	125
H ₂ Se	91	91	1.47	1.47	122	125
H ₂ S	93	92	1.34	1.34	122	125
PH ₃	99	93	1.41	1.41	121	125
COF ₂	125	126	1.19	1.17	122	125
CH ₃ F	105	109	1.09	1.09	121	125
HCHO	119	121	1.22	1.20	120	125
(CH ₃) ₂ O	114	111	1.43	1.40	122	125
CH ₃ NH ₂	107	115	1.48	1.46	120	125

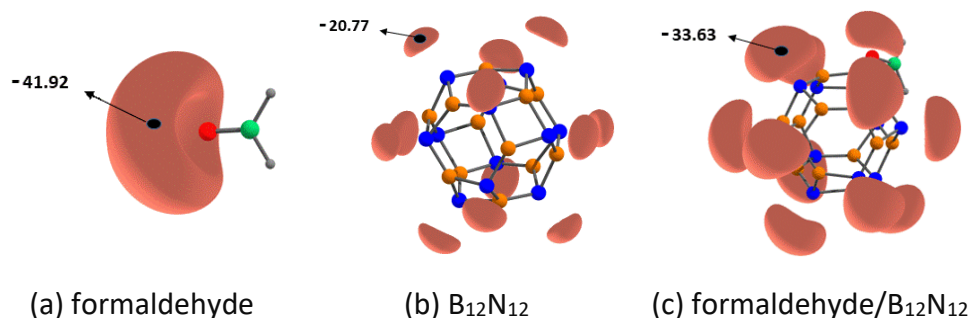


Figure S1. MESP plots of (a) formaldehyde (where position of $V_{\min-x}$ is noted), (b) $B_{12}N_{12}$ cage (where position of $V_{\min-c}$ is noted), and (c) formaldehyde-adsorbed $B_{12}N_{12}$ (where position of $V_{\min-c}$ is noted) with -0.0235 a.u. isosurface. Color code: orange-B, blue-N, green-C, red-O and gray-H.

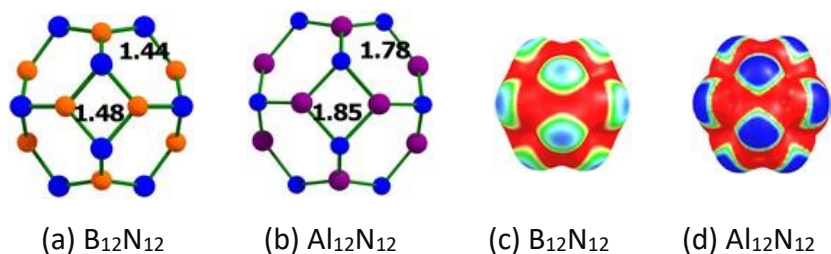


Figure S2. Optimized structures of (a) $B_{12}N_{12}$ and (b) $Al_{12}N_{12}$.^{S1} The bond distances are given in Å. Color code: purple-Al, orange-B, and blue-N. Also shown are the MESP mapped onto the 0.01 a.u. electron density isosurface of (c) $B_{12}N_{12}$ and (d) $Al_{12}N_{12}$.^{S1} Color code: blue -0.04 a.u. to red 0.04 a.u. Blue represents the most electron-rich region and red the most electron-poor region.

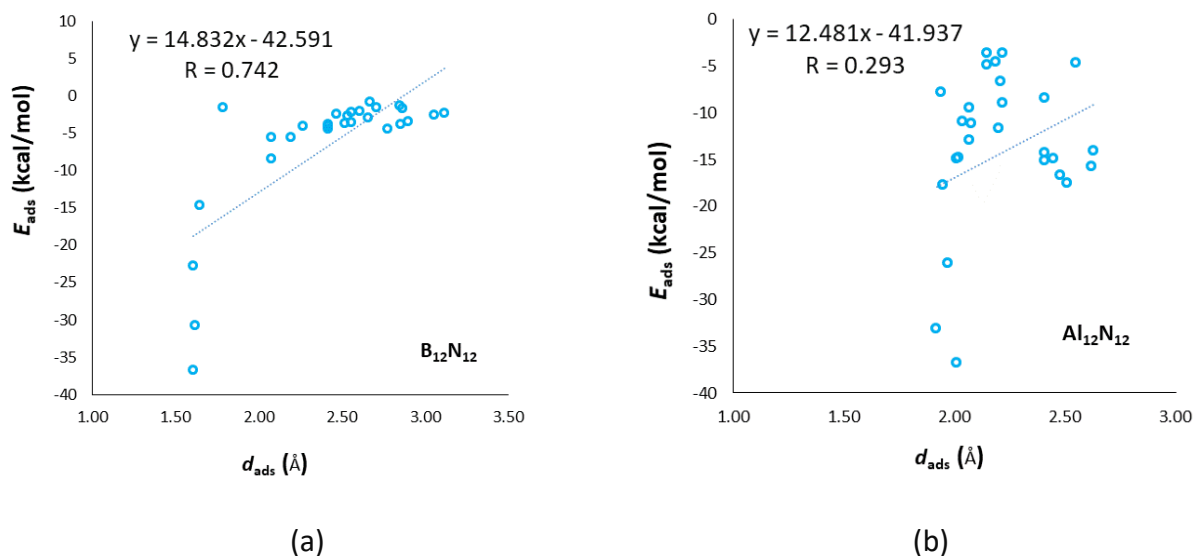
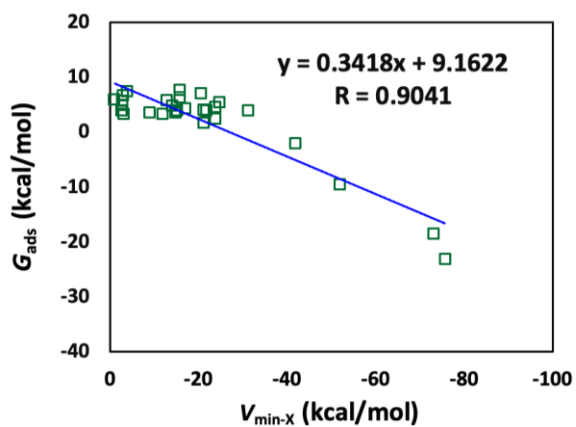
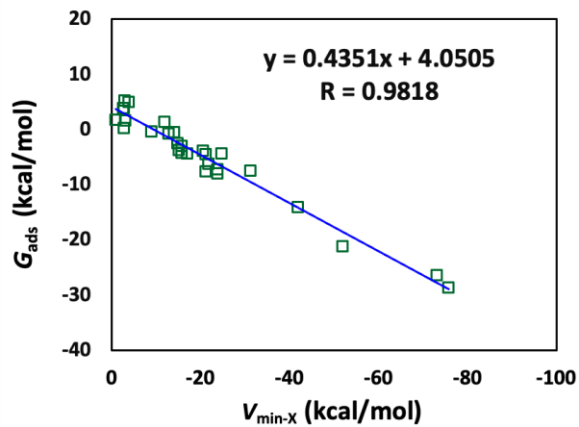


Figure S3. Correlation between d_{ads} and E_{ads} for gas-adsorbed (a) $B_{12}N_{12}$ and (b) $Al_{12}N_{12}$ nanocages.

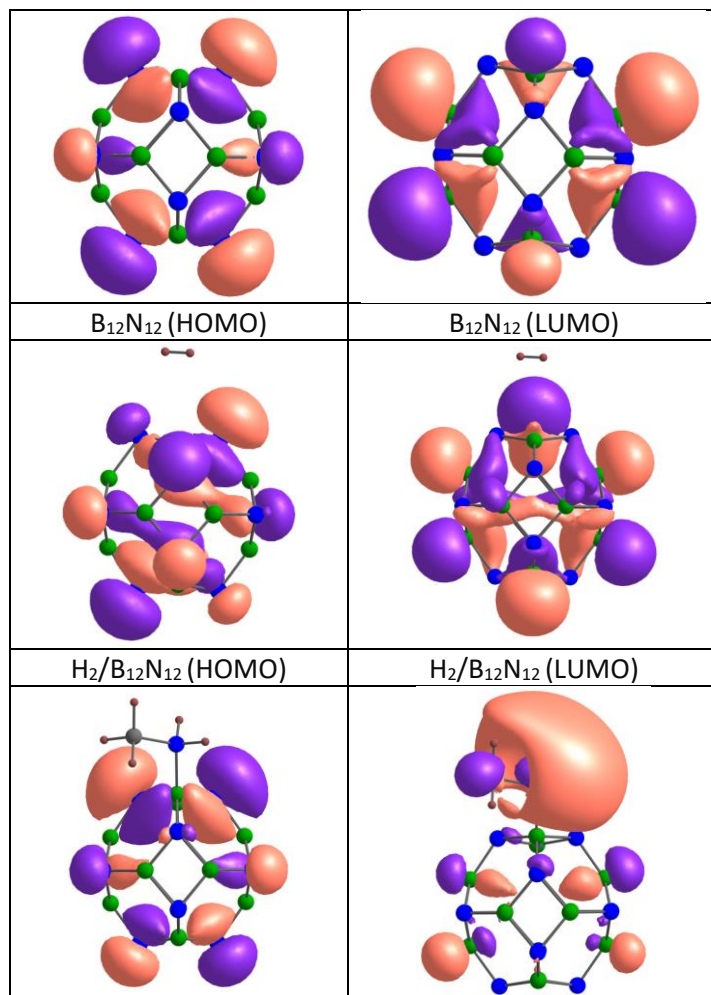


(a)



(b)

Figure S4. Correlation between $V_{\min-X}$ and G_{ads} for gas-adsorbed (a) $B_{12}N_{12}$ and (b) $Al_{12}N_{12}$ nanocages.



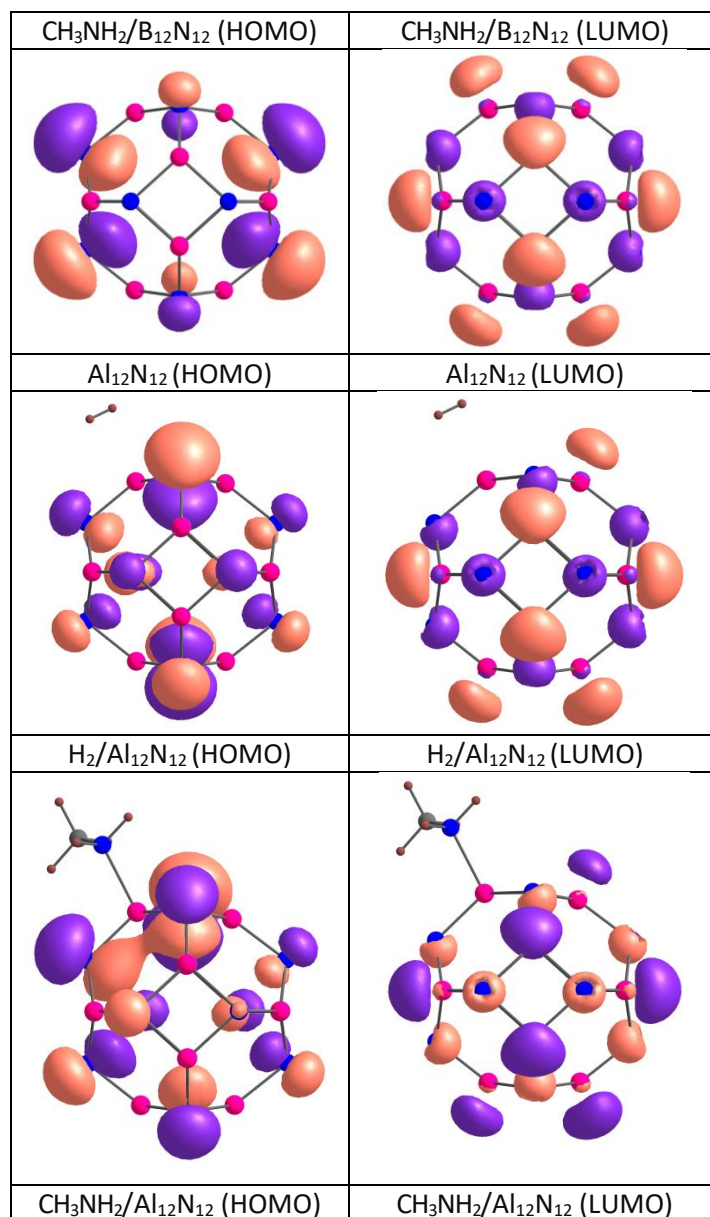
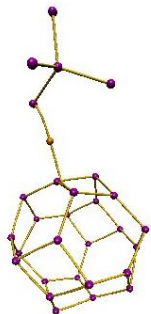
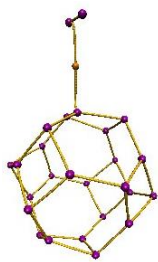


Figure S5. Molecular orbital diagrams for the pristine nanocages and some representative gas-adsorbed systems



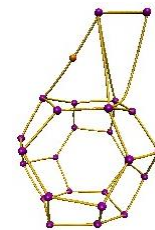
(a) $\text{SiH}_4/\text{B}_{12}\text{N}_{12}$



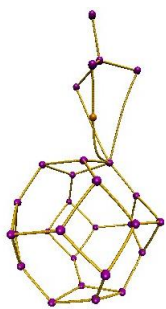
(b) $\text{H}_2/\text{B}_{12}\text{N}_{12}$



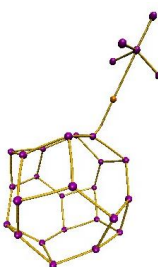
(c) $\text{Cl}_2/\text{B}_{12}\text{N}_{12}$



(d) $\text{F}_2/\text{B}_{12}\text{N}_{12}$



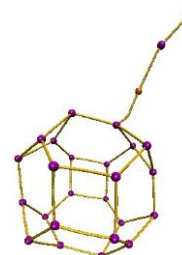
(e) $\text{CF}_4/\text{B}_{12}\text{N}_{12}$



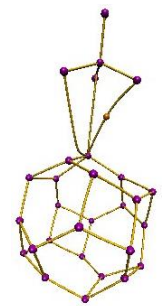
(f) $\text{CH}_4/\text{B}_{12}\text{N}_{12}$



(g) $\text{CF}_2\text{Cl}_2/\text{B}_{12}\text{N}_{12}$



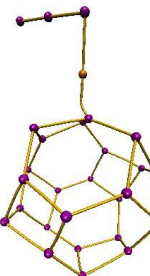
(h) $\text{N}_2/\text{B}_{12}\text{N}_{12}$



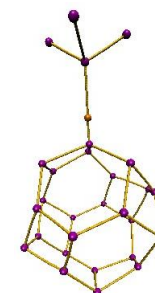
(i) $\text{CHF}_3/\text{B}_{12}\text{N}_{12}$



(j) $\text{OCS}/\text{B}_{12}\text{N}_{12}$



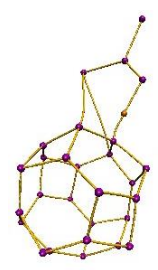
(k) $\text{N}_2\text{O}/\text{B}_{12}\text{N}_{12}$



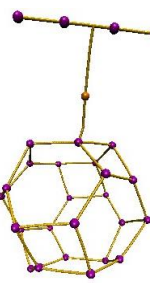
(l) $\text{AsH}_3/\text{B}_{12}\text{N}_{12}$



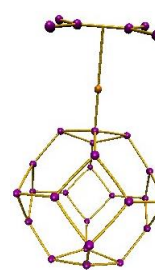
(m) $\text{CH}_3\text{Cl}/\text{B}_{12}\text{N}_{12}$



(n) $\text{COCl}_2/\text{B}_{12}\text{N}_{12}$



(o) $\text{C}_2\text{H}_2/\text{B}_{12}\text{N}_{12}$



(p) $\text{C}_2\text{H}_4/\text{B}_{12}\text{N}_{12}$

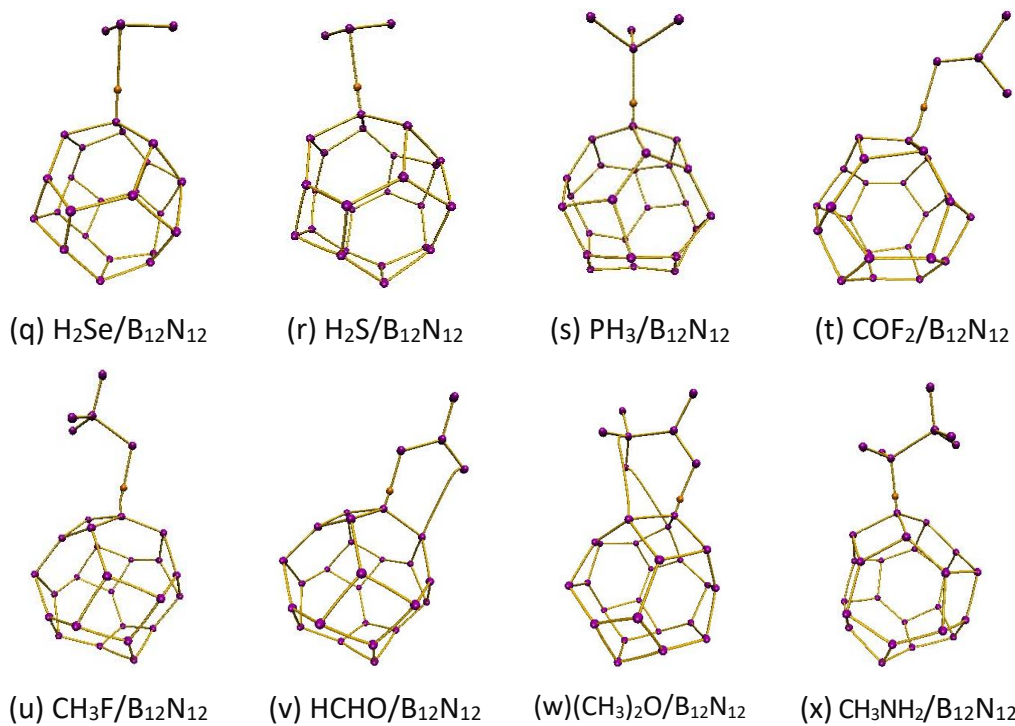
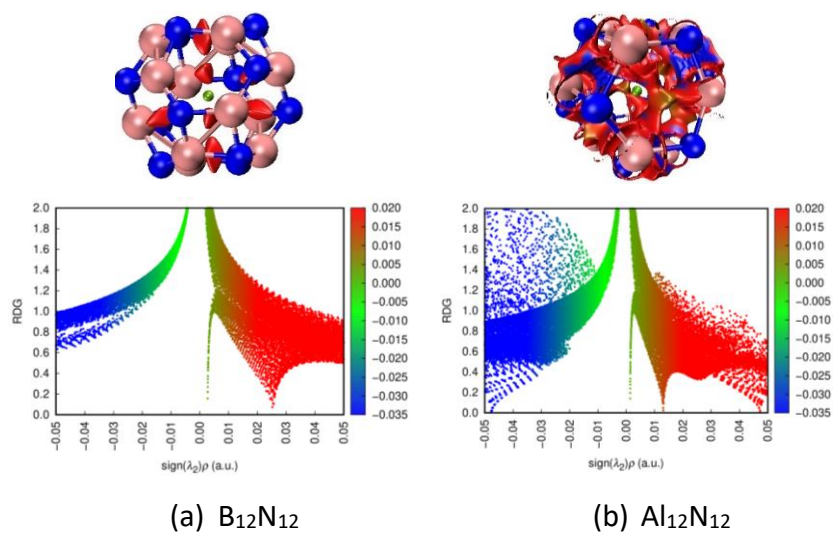


Figure S6. QTAIM plots for (a) SiH_4 , (b) H_2 , (c) Cl_2 , (d) F_2 , (e) CF_4 , (f) CH_4 , (g) CF_2Cl_2 , (h) N_2 , (i) CHF_3 , (j) OCS , (k) N_2O , (l) AsH_3 , (m) CH_3Cl , (n) COCl_2 , (o) C_2H_2 , (p) C_2H_4 , (q) H_2Se , (r) H_2S , (s) PH_3 , (t) COF_2 , (u) CH_3F , (v) HCHO , (w) $(\text{CH}_3)_2\text{O}$, and (x) CH_3NH_2 adsorbed on $\text{B}_{12}\text{N}_{12}$.



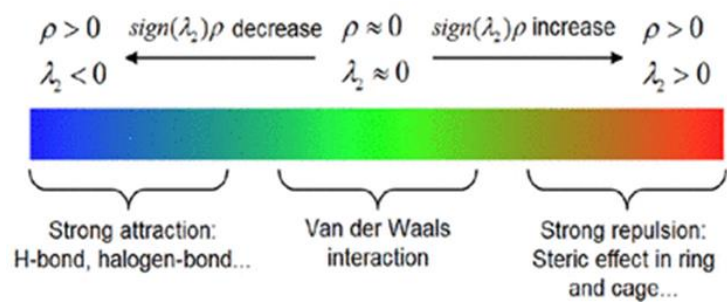
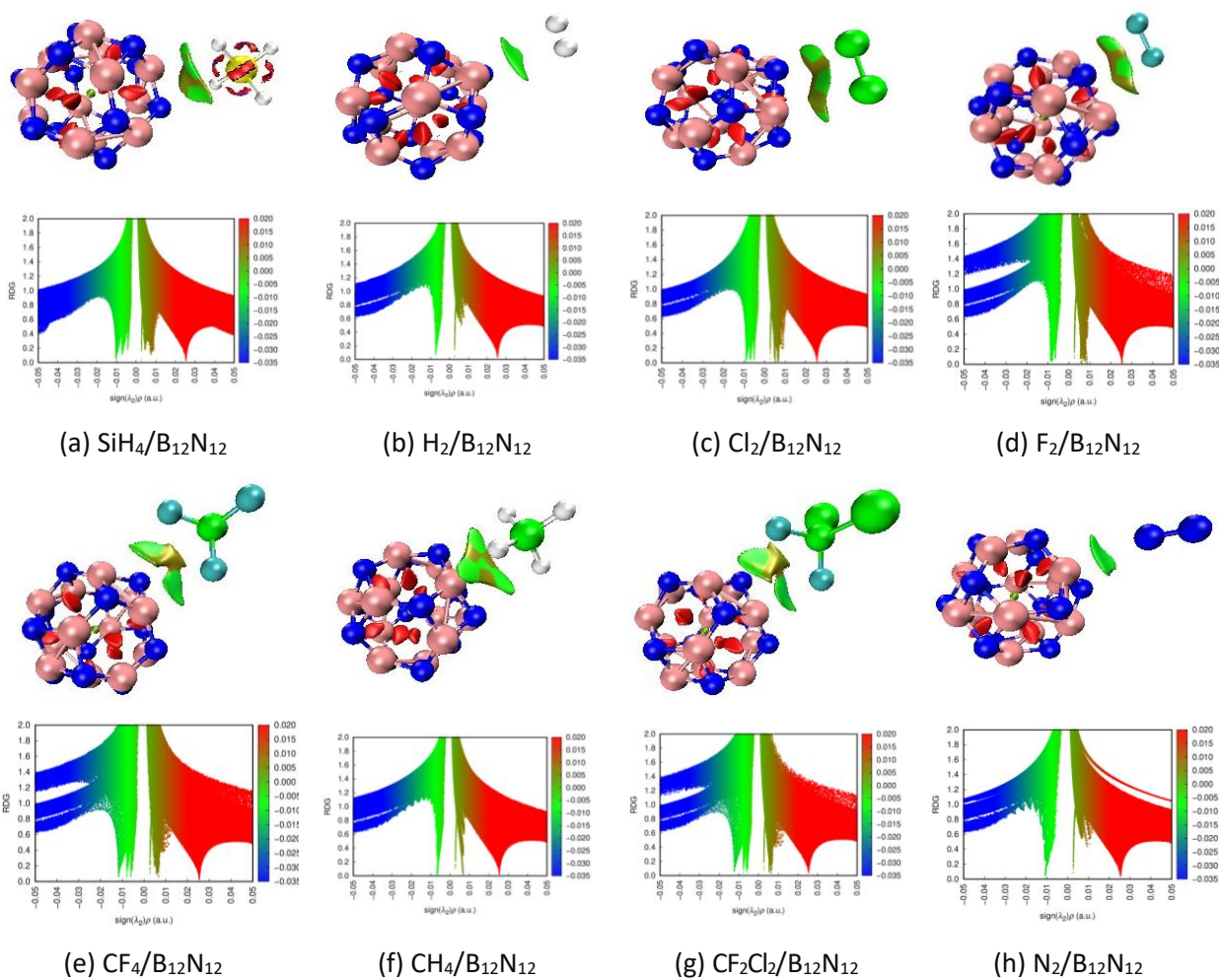
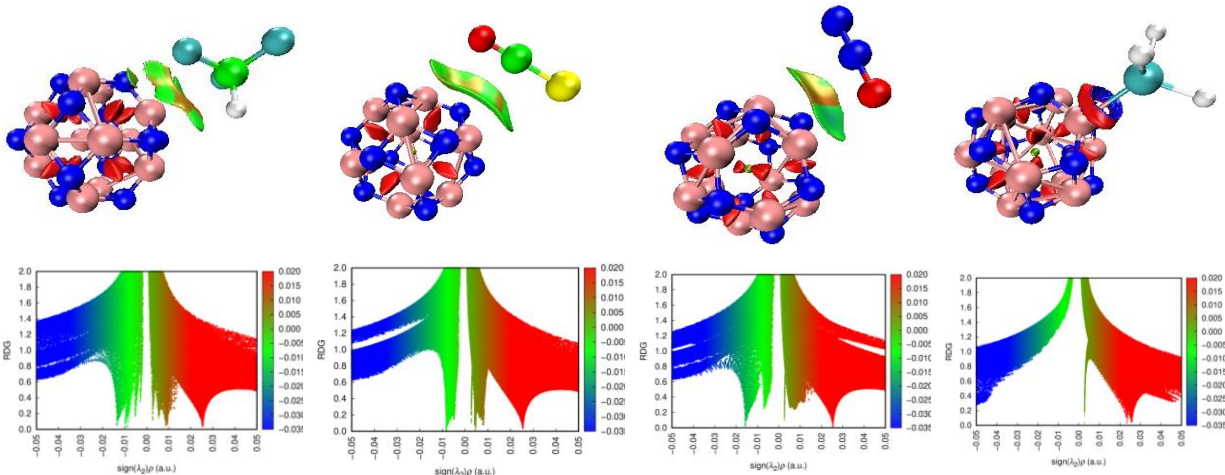


Figure S7. The NCI iso-surface plots with the complementary 2D NCI diagrams for (a) $B_{12}N_{12}$ and (b) $Al_{12}N_{12}$.



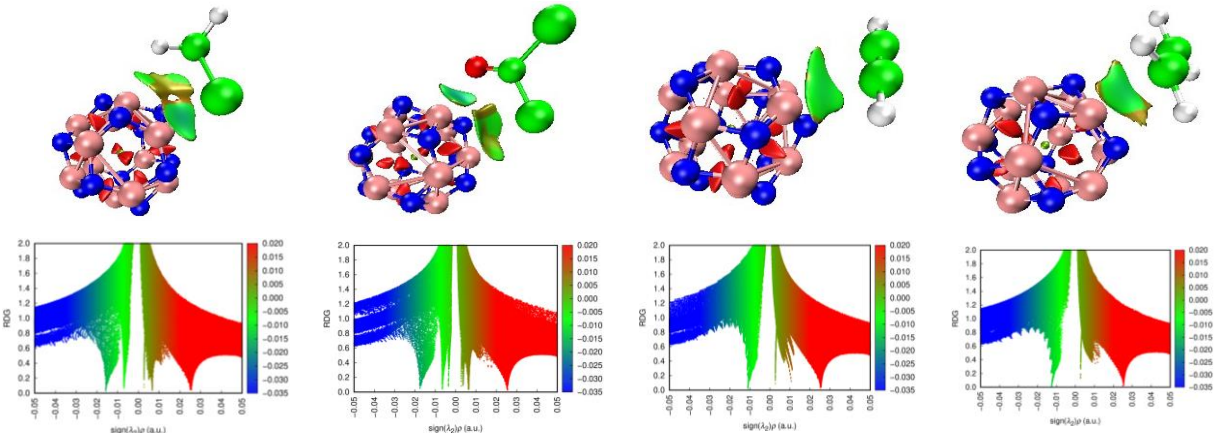


(i) $\text{CHF}_3/\text{B}_{12}\text{N}_{12}$

(j) $\text{OCS}/\text{B}_{12}\text{N}_{12}$

(k) $\text{N}_2\text{O}/\text{B}_{12}\text{N}_{12}$

(l) $\text{AsH}_3/\text{B}_{12}\text{N}_{12}$

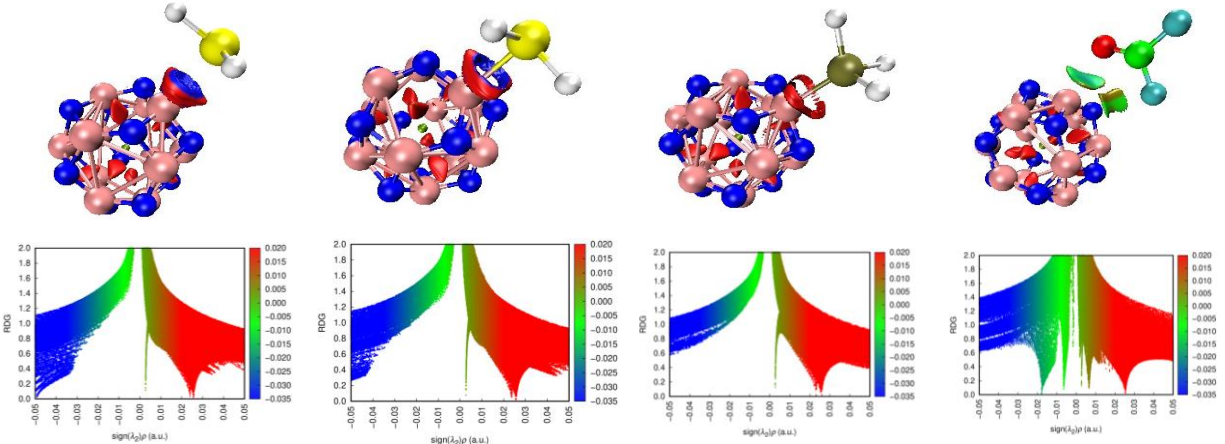


(m) $\text{CH}_3\text{Cl}/\text{B}_{12}\text{N}_{12}$

(n) $\text{COCl}_2/\text{B}_{12}\text{N}_{12}$

(o) $\text{C}_2\text{H}_2/\text{B}_{12}\text{N}_{12}$

(p) $\text{C}_2\text{H}_4/\text{B}_{12}\text{N}_{12}$



(q) $\text{H}_2\text{Se}/\text{B}_{12}\text{N}_{12}$

(r) $\text{H}_2\text{S}/\text{B}_{12}\text{N}_{12}$

(s) $\text{PH}_3/\text{B}_{12}\text{N}_{12}$

(t) $\text{COF}_2/\text{B}_{12}\text{N}_{12}$

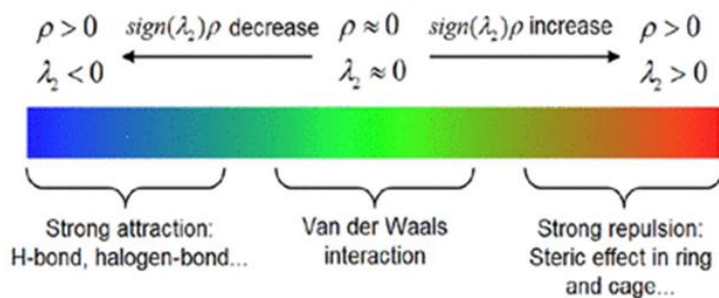
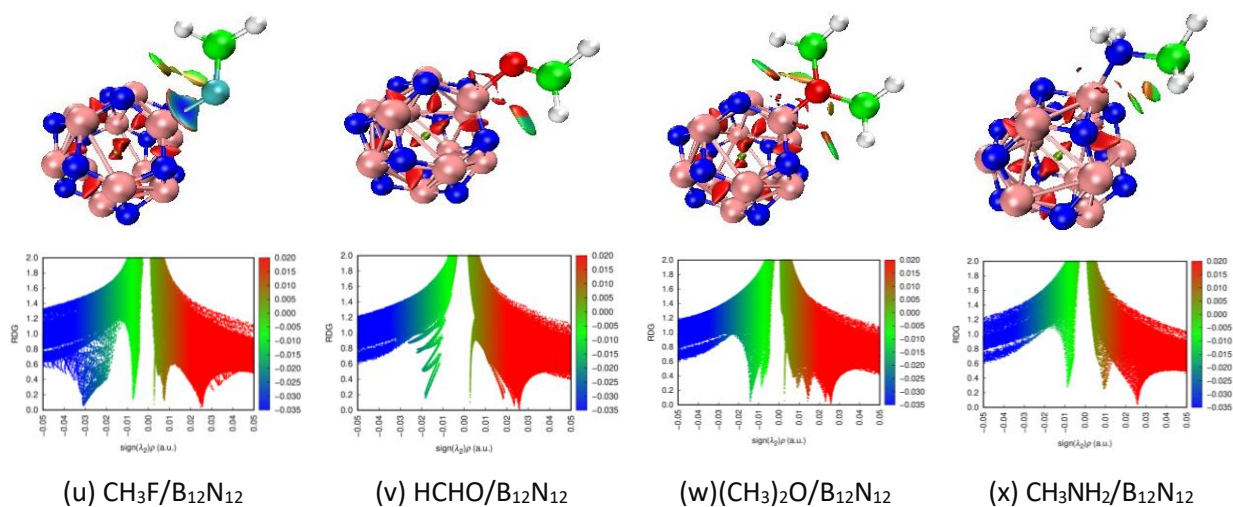
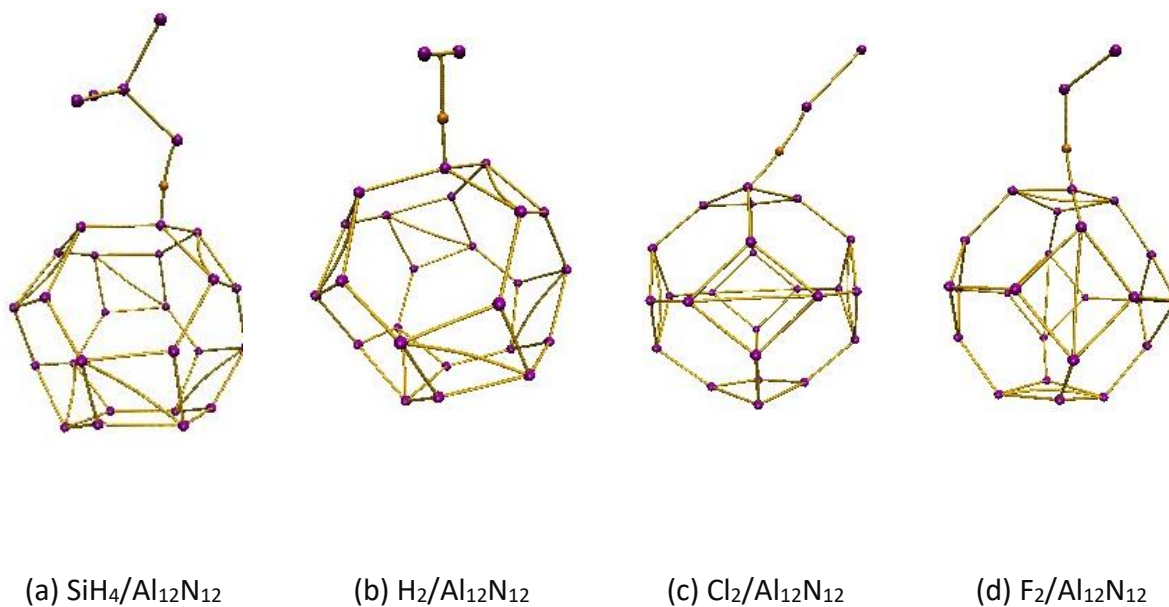
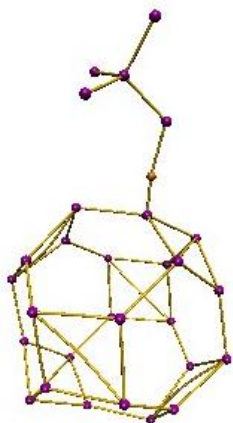
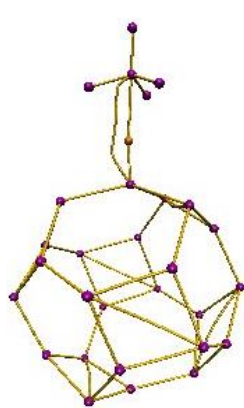


Figure S8. The NCI isosurface plots with the complementary 2D NCI diagrams for the gases adsorbed on B₁₂N₁₂.





(e) $\text{CF}_4/\text{Al}_{12}\text{N}_{12}$



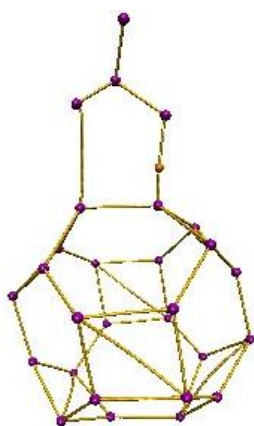
(f) $\text{CH}_4/\text{Al}_{12}\text{N}_{12}$



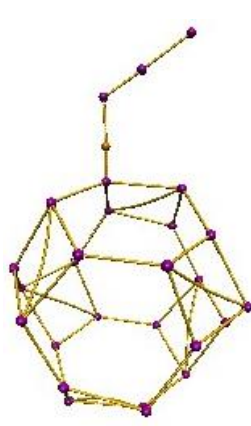
(g) $\text{CF}_2\text{Cl}_2/\text{Al}_{12}\text{N}_{12}$



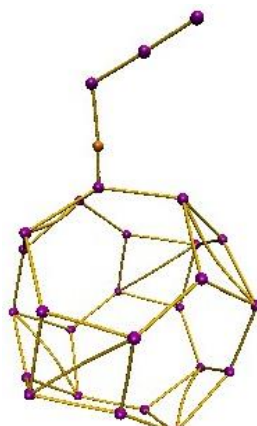
(h) $\text{N}_2/\text{Al}_{12}\text{N}_{12}$



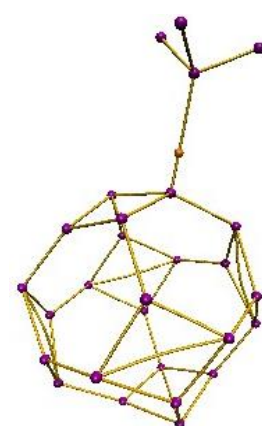
(i) $\text{CHF}_3/\text{Al}_{12}\text{N}_{12}$



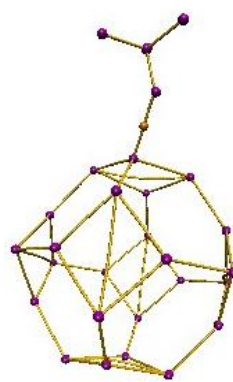
(j) $\text{OCS}/\text{Al}_{12}\text{N}_{12}$



(k) $\text{N}_2\text{O}/\text{Al}_{12}\text{N}_{12}$



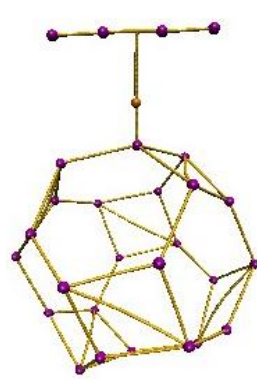
(l) $\text{AsH}_3/\text{Al}_{12}\text{N}_{12}$



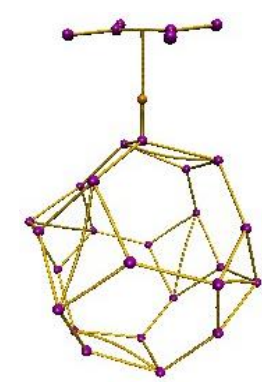
(m) $\text{CH}_3\text{Cl}/\text{Al}_{12}\text{N}_{12}$



(n) $\text{COCl}_2/\text{Al}_{12}\text{N}_{12}$



(o) $\text{C}_2\text{H}_2/\text{Al}_{12}\text{N}_{12}$



(p) $\text{C}_2\text{H}_4/\text{Al}_{12}\text{N}_{12}$

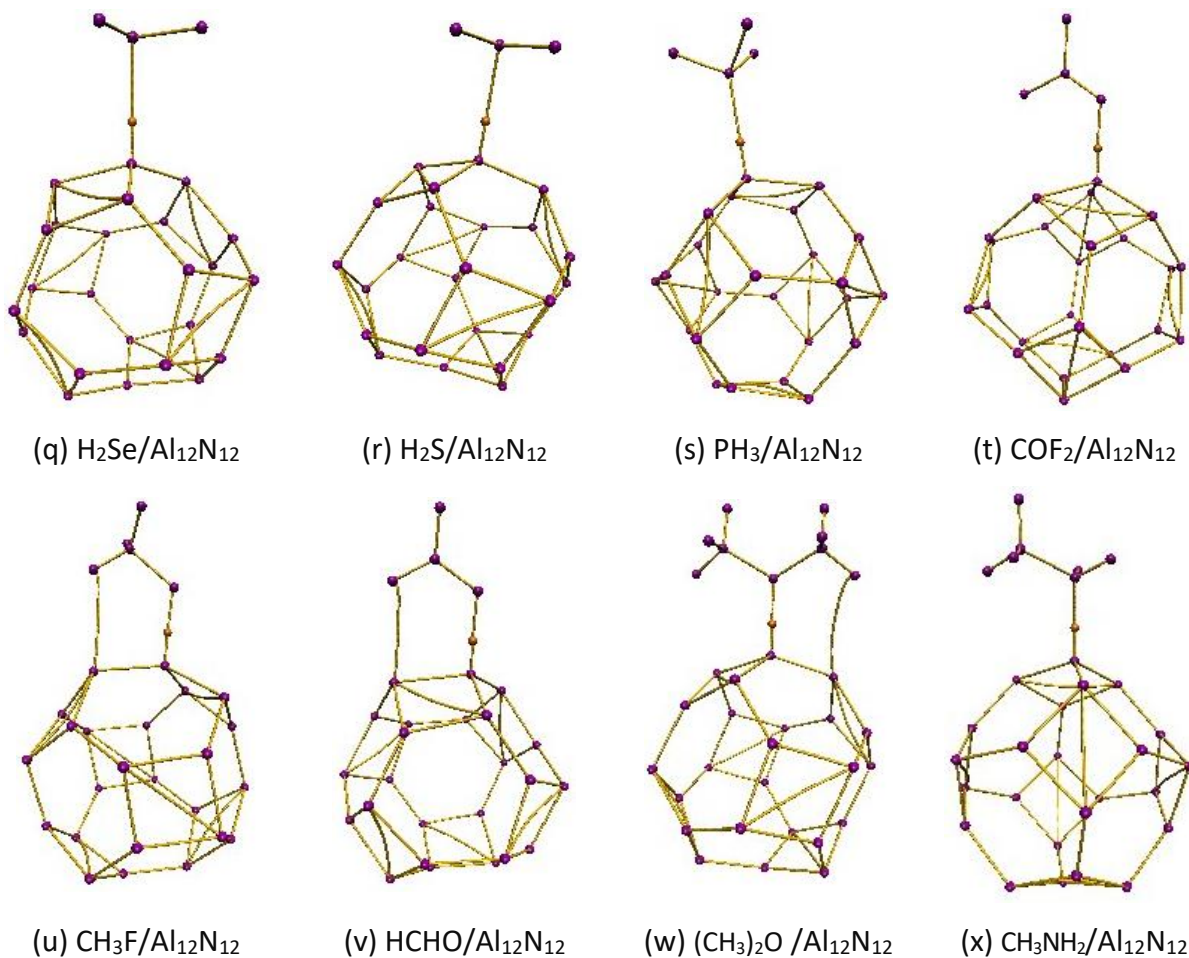
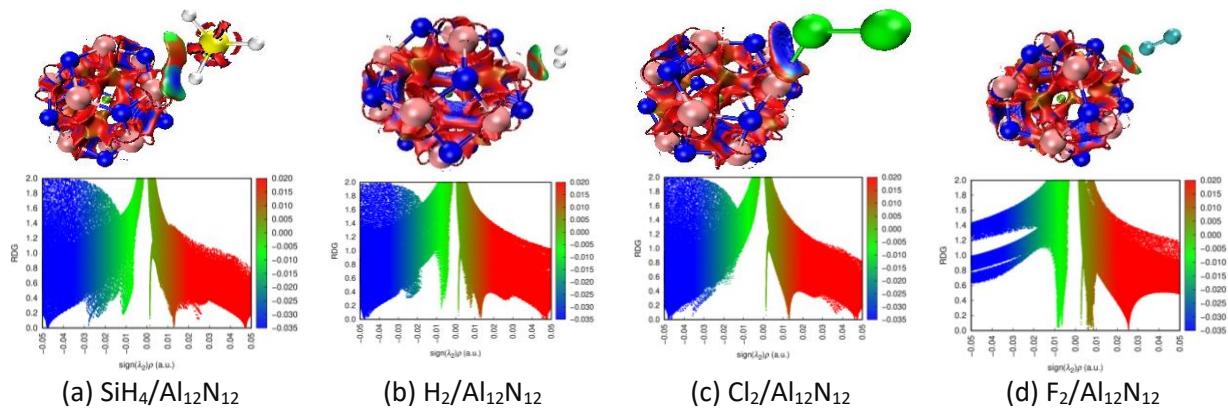
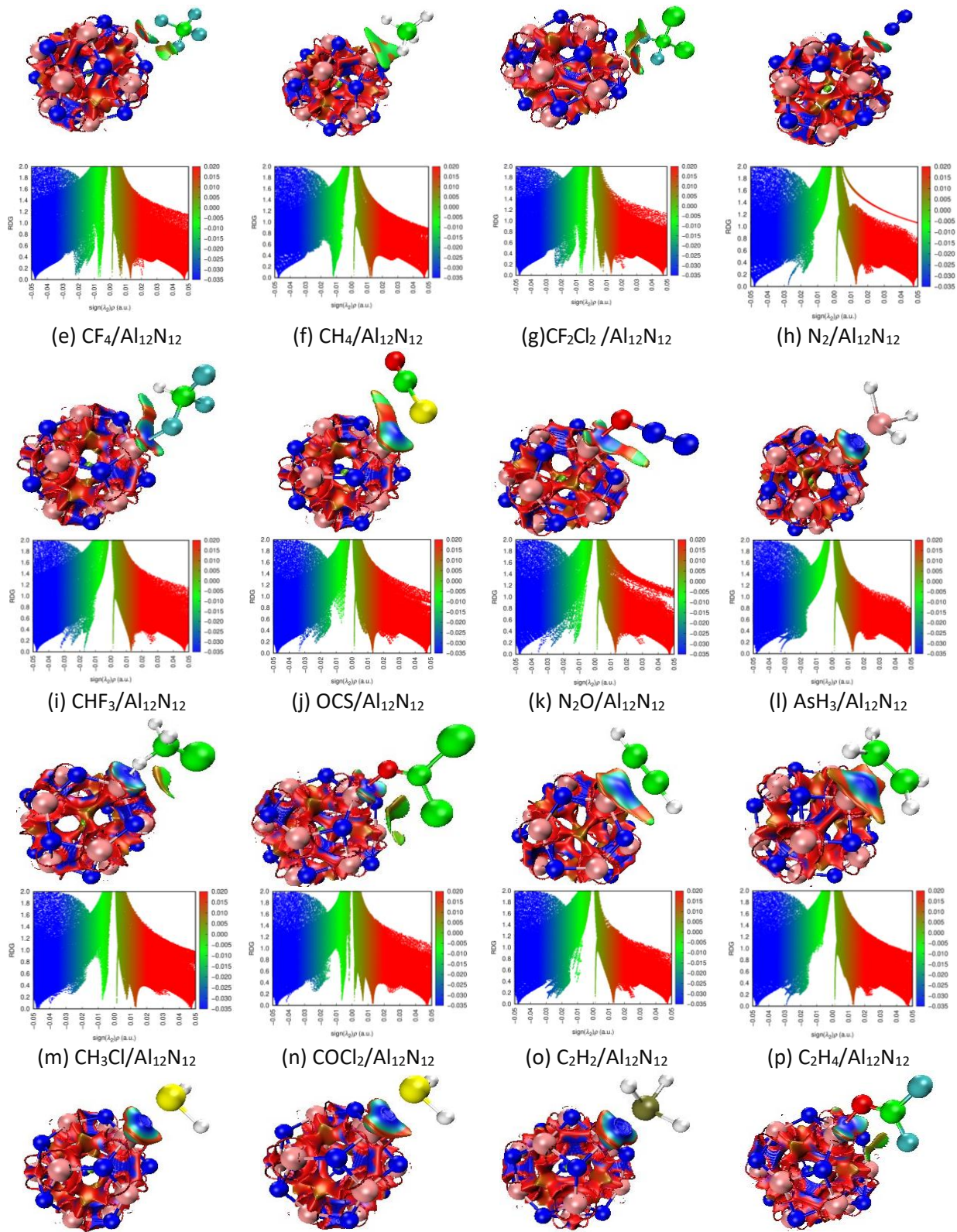


Figure S9. QAIM plots for (a) SiH_4 , (b) H_2 , (c) Cl_2 , (d) F_2 , (e) CF_4 , (f) CH_4 , (g) CF_2Cl_2 , (h) N_2 , (i) CHF_3 , (j) OCS , (k) N_2O , (l) AsH_3 , (m) CH_3Cl , (n) COCl_2 , (o) C_2H_2 , (p) C_2H_4 , (q) H_2Se , (r) H_2S , (s) PH_3 , (t) COF_2 , (u) CH_3F , (v) HCHO , (w) $(\text{CH}_3)_2\text{O}$, and (x) CH_3NH_2 adsorbed on $\text{Al}_{12}\text{N}_{12}$.





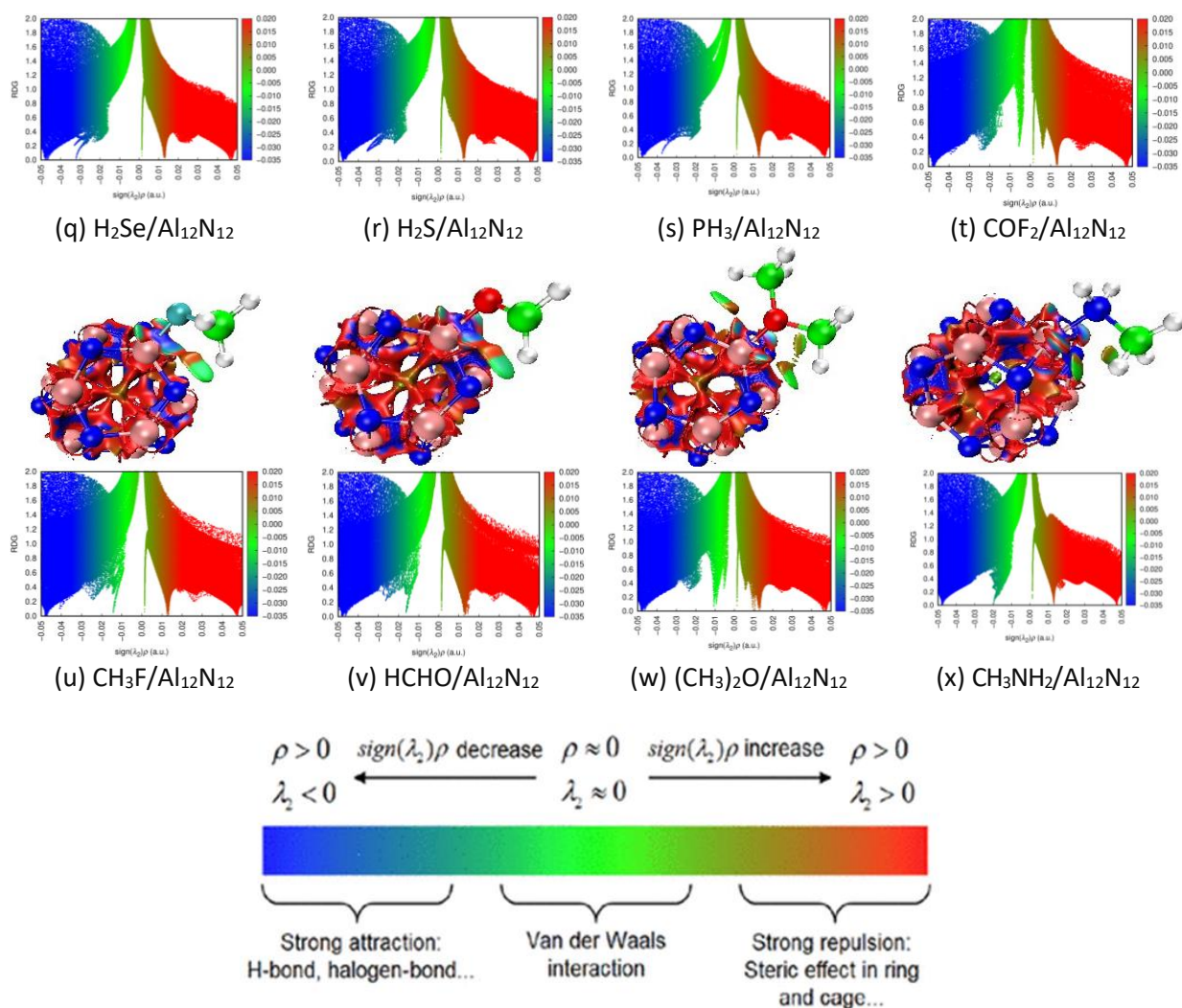


Figure S10. The NCI isosurface plots with the complementary 2D NCI diagrams for the gases adsorbed on $\text{Al}_{12}\text{N}_{12}$.

Table S3. Cartesian coordinates for the gas-adsorbed $\text{B}_{12}\text{N}_{12}$ nanocages

$\text{SiH}_4/\text{B}_{12}\text{N}_{12}$				$\text{H}_2/\text{B}_{12}\text{N}_{12}$			
5	1.498434000	-0.589584000	0.179243000	5	1.367578000	0.638163000	-1.512161000
5	1.114597000	1.261982000	0.463102000	5	2.115720000	-0.092781000	0.084878000
7	1.308978000	0.167381000	1.441807000	7	1.861793000	-0.730475000	-1.230028000
7	1.610648000	0.565342000	-0.749957000	7	1.913385000	1.321843000	-0.315219000
7	0.908070000	-1.863346000	-0.133184000	7	0.141990000	0.969861000	-2.186711000
7	-1.275330000	-2.249634000	-0.500315000	7	-1.927592000	0.656792000	-1.367960000
5	-0.341485000	-2.068132000	0.637030000	5	-0.851612000	-0.119012000	-2.030379000
5	-0.088564000	-1.731071000	-1.221295000	5	-0.807999000	1.621786000	-1.253896000
5	-2.318360000	-1.261674000	-0.463078000	5	-2.243306000	0.091937000	-0.084469000
5	-2.694520000	0.585731000	-0.178580000	5	-1.500542000	-0.638417000	1.512972000
7	-2.812585000	-0.564818000	0.748588000	7	-2.046205000	-1.321775000	0.315477000
7	-2.514313000	-0.166673000	-1.443332000	7	-1.995066000	0.730435000	1.230606000
7	0.071053000	2.250027000	0.500511000	7	1.794879000	-0.657045000	1.368007000

7	-2.112044000	1.862248000	0.133072000	7	-0.274966000	-0.969969000	2.186499000
5	-1.115161000	1.731013000	1.222431000	5	0.675135000	-1.621408000	1.253478000
5	-0.862054000	2.068806000	-0.636551000	5	0.719047000	0.118844000	2.029756000
5	0.063699000	-0.183788000	2.067233000	5	0.766674000	-1.656613000	-1.145209000
7	-0.661967000	-1.465059000	1.901730000	7	-0.552625000	-1.506769000	-1.805174000
5	-1.788347000	-0.511792000	1.755683000	5	-0.989195000	-1.922986000	-0.451005000
7	-1.105543000	0.712621000	2.236528000	7	0.322458000	-2.368531000	0.077069000
5	0.583955000	0.511425000	-1.755054000	5	0.856062000	1.922167000	0.450668000
7	-0.098501000	-0.712873000	-2.236343000	7	-0.455565000	2.368194000	-0.077126000
5	-1.267816000	0.183288000	-2.068239000	5	-0.899663000	1.657113000	1.145537000
7	-0.541824000	1.464912000	-1.901221000	7	0.419598000	1.506590000	1.805084000
14	4.813549000	0.003453000	-0.001149000	1	4.807490000	-0.363406000	-0.015384000
1	4.277172000	1.197940000	0.686129000	1	4.738426000	0.375370000	0.010869000
1	3.906908000	-1.148630000	0.232666000				
1	6.142100000	-0.329709000	0.555758000				
1	4.925731000	0.250147000	-1.453285000				
Cl ₂ /B ₁₂ N ₁₂				F ₂ /B ₁₂ N ₁₂			
5	-0.006094000	-1.235938000	1.531259000	5	0.323340000	1.278569000	-1.559210000
5	1.039460000	-0.906575000	-0.030761000	5	1.401252000	1.060665000	-0.000075000
7	1.057976000	-0.233736000	1.291505000	7	1.468080000	0.372012000	-1.311451000
7	0.212003000	-2.082067000	0.333022000	7	0.478999000	2.159827000	-0.376896000
7	-1.269685000	-0.985395000	2.169490000	7	-0.919445000	0.914611000	-2.183200000
7	-2.950159000	0.234118000	1.309075000	7	-2.488528000	-0.423354000	-1.289447000
5	-1.661187000	0.436024000	2.013000000	5	-1.191811000	-0.531268000	-2.000050000
5	-2.381962000	-1.131152000	1.200886000	5	-2.033699000	0.985468000	-1.208403000
5	-2.937776000	0.891279000	0.030893000	5	-2.414167000	-1.055001000	-0.000413000
5	-1.897287000	1.223932000	-1.532008000	5	-1.339809000	-1.273207000	1.559869000
7	-2.113512000	2.068675000	-0.332990000	7	-1.493581000	-2.154025000	0.377293000
7	-2.963084000	0.221530000	-1.291161000	7	-2.485946000	-0.366139000	1.310272000
7	1.045238000	-0.246411000	-1.308890000	7	1.470595000	0.429386000	1.290020000
7	-0.633856000	0.973784000	-2.169632000	7	-0.097343000	-0.909331000	2.183369000
5	0.479278000	1.118684000	-1.200649000	5	1.018293000	-0.979334000	1.208480000
5	-0.242434000	-0.447816000	-2.012789000	5	0.174948000	0.536675000	1.999803000
5	0.503033000	1.088229000	1.200536000	5	1.023815000	-0.989306000	-1.193454000
7	-0.762629000	1.542404000	1.825012000	7	-0.204410000	-1.556686000	-1.800226000
5	-0.923074000	2.122658000	0.470723000	5	-0.307891000	-2.124022000	-0.434583000
7	0.465151000	1.935110000	-0.016674000	7	1.062844000	-1.814155000	0.038376000
5	-0.978537000	-2.134377000	-0.470990000	5	-0.706742000	2.129580000	0.434988000
7	-2.366173000	-1.945720000	0.016845000	7	-2.077422000	1.819458000	-0.038601000
5	-2.405500000	-1.100402000	-1.200353000	5	-2.039291000	0.995191000	1.193011000
7	-1.140469000	-1.554433000	-1.825595000	7	-0.812096000	1.562383000	1.800752000
17	3.901462000	1.027654000	0.001288000	9	3.908975000	-0.690335000	-0.000678000
17	4.157056000	-0.975756000	-0.001216000	9	4.218423000	0.645006000	0.000495000
CF ₄ /B ₁₂ N ₁₂				CH ₄ /B ₁₂ N ₁₂			
5	0.854940000	-0.648655000	0.286451000	5	1.848599000	0.061150000	-0.024319000
5	0.551662000	1.236719000	0.340218000	5	1.057833000	-1.581194000	0.544662000
7	0.686171000	0.259465000	1.446206000	7	1.595087000	-1.190408000	-0.780323000
7	1.029891000	0.379319000	-0.771659000	7	1.598003000	-0.455812000	1.344023000
7	0.218038000	-1.926398000	0.117597000	7	1.556014000	1.392780000	-0.484198000
7	-1.975484000	-2.264133000	-0.240630000	7	-0.493898000	2.265150000	-0.782952000
5	-1.049455000	-1.986466000	0.883630000	5	0.463873000	1.377809000	-1.485820000
5	-0.757858000	-1.884475000	-0.996874000	5	0.466222000	2.000889000	0.315467000
5	-2.975385000	-1.236349000	-0.339954000	5	-1.735995000	1.582238000	-0.544991000
5	-3.274476000	0.646182000	-0.284600000	5	-2.518197000	-0.061130000	0.024186000
7	-3.454090000	-0.379143000	0.770907000	7	-2.275833000	0.455979000	-1.343933000
7	-3.110975000	-0.259475000	-1.447026000	7	-2.273040000	1.190430000	0.780205000
7	-0.448496000	2.264624000	0.240601000	7	-0.184241000	-2.265011000	0.782817000
7	-2.641554000	1.925918000	-0.117273000	7	-2.234238000	-1.392967000	0.484142000

5	-1.665446000	1.884960000	0.997684000	5	-1.144162000	-2.001566000	-0.315695000
5	-1.373828000	1.986620000	-0.883755000	5	-1.141829000	-1.378230000	1.486298000
5	-0.581353000	0.039074000	2.085494000	5	0.528176000	-1.010135000	-1.725852000
7	-1.359722000	-1.222377000	2.061143000	7	0.118989000	0.275093000	-2.340949000
5	-2.441516000	-0.247998000	1.782683000	5	-1.211085000	-0.270934000	-1.979434000
7	-1.712716000	0.996318000	2.126338000	7	-0.802494000	-1.661815000	-1.669828000
5	0.017342000	0.247888000	-1.782329000	5	0.533180000	0.270919000	1.978623000
7	-0.711446000	-0.996198000	-2.126274000	7	0.124528000	1.661914000	1.669916000
5	-1.842603000	-0.039110000	-2.086230000	5	-1.206145000	1.010578000	1.726470000
7	-1.064365000	1.222464000	-2.061178000	7	-0.796952000	-0.275120000	2.340752000
6	4.156269000	0.005046000	-0.005049000	6	4.876241000	-0.000424000	0.000528000
9	3.656176000	1.095307000	0.539017000	1	4.518780000	-0.779092000	-0.673614000
9	5.396712000	-0.158410000	0.402582000	1	4.511121000	0.971587000	-0.332918000
9	3.437575000	-1.042652000	0.374987000	1	5.965353000	0.006382000	-0.004092000
9	4.127925000	0.102988000	-1.313594000	1	4.521479000	-0.199812000	1.011786000
CF ₂ Cl ₂ /B ₁₂ N ₁₂				N ₂ /B ₁₂ N ₁₂			
5	0.453209000	-0.336967000	-0.555717000	5	-1.707746000	-0.157167000	-0.000273000
5	0.094919000	-0.159419000	1.312633000	5	-0.983767000	1.612389000	0.002544000
7	0.277909000	-1.376453000	0.487277000	7	-1.489565000	0.791152000	-1.122244000
7	0.576096000	0.845893000	0.334614000	7	-1.489582000	0.787592000	1.124710000
7	-0.151893000	-0.344789000	-1.860203000	7	-1.351242000	-1.551730000	-0.002470000
7	-2.341103000	-0.081431000	-2.297499000	7	0.736122000	-2.386575000	-0.003775000
5	-1.402003000	-1.140467000	-1.855312000	5	-0.248142000	-1.816180000	-0.955068000
5	-1.149534000	0.743683000	-1.984736000	5	-0.248155000	-1.819199000	0.949298000
5	-3.371526000	0.124376000	-1.317099000	5	1.946951000	-1.612742000	-0.002543000
5	-3.724038000	0.300115000	0.548768000	5	2.655906000	0.157607000	0.000274000
7	-3.854104000	-0.879919000	-0.339106000	7	2.451458000	-0.785600000	-1.125034000
7	-3.556691000	1.342549000	-0.492188000	7	2.451438000	-0.789165000	1.122572000
7	-0.936224000	0.046621000	2.293658000	7	0.226727000	2.389041000	0.003776000
7	-3.125107000	0.309679000	1.855308000	7	2.313612000	1.553702000	0.002469000
5	-2.126798000	-0.779454000	1.981161000	5	1.209927000	1.822894000	-0.950350000
5	-1.874397000	1.105813000	1.851483000	5	1.209917000	1.819874000	0.956127000
5	-0.969813000	-2.066761000	0.316815000	5	-0.404408000	0.358778000	-1.958016000
7	-1.712489000	-2.219251000	-0.957342000	7	0.063243000	-1.038347000	-2.123265000
5	-2.826671000	-1.844267000	-0.054522000	5	1.365877000	-0.349842000	-1.960731000
7	-2.127561000	-2.012080000	1.241906000	7	0.898735000	1.048029000	-2.120074000
5	-0.451328000	1.808245000	0.050247000	5	-0.404440000	0.352570000	1.959120000
7	-1.150272000	1.977204000	-1.246088000	7	0.063210000	-1.045065000	2.119962000
5	-2.307646000	2.033034000	-0.321347000	5	1.365841000	-0.356058000	1.959632000
7	-1.565529000	2.184607000	0.953159000	7	0.898706000	1.041310000	2.123384000
6	3.773262000	-0.102919000	0.043551000	7	-4.414307000	-0.144214000	-0.000165000
9	3.182569000	-0.431187000	1.183738000	7	-5.471240000	0.120639000	0.000143000
9	2.980570000	-0.499339000	-0.956414000				
17	5.305697000	-0.964163000	-0.079523000				
17	3.978955000	1.640879000	-0.037157000				
CHF ₃ /B ₁₂ N ₁₂				OCS/B ₁₂ N ₁₂			
5	1.060602000	-0.750204000	-0.247172000	5	-1.061039000	2.099255000	-0.480365000
5	0.224390000	-1.107392000	1.437170000	5	0.471135000	1.220168000	-1.198540000
7	0.368255000	-1.966337000	0.240857000	7	-0.832838000	1.534085000	-1.832209000
7	1.178510000	-0.035431000	1.058264000	7	0.335006000	2.060660000	0.013391000
7	0.857747000	-0.126893000	-1.525243000	7	-2.242544000	1.923197000	0.319480000
7	-1.000603000	0.936742000	-2.206196000	7	-2.894531000	0.000271000	1.282679000
5	-0.482162000	-0.445655000	-2.067602000	5	-2.935213000	0.663837000	-0.042637000
5	0.204495000	1.192987000	-1.379055000	5	-1.941819000	1.110800000	1.522615000
5	-2.196373000	1.108483000	-1.428945000	5	-2.199681000	-1.254819000	1.200091000
5	-3.019277000	0.744553000	0.252873000	5	-0.669879000	-2.136184000	0.480143000
7	-3.144815000	0.035757000	-1.042499000	7	-2.066948000	-2.096876000	-0.013147000
7	-2.338843000	1.969773000	-0.229781000	7	-0.895834000	-1.569956000	1.831560000

7	-0.970201000	-0.936068000	2.217236000	7	1.165655000	-0.036679000	-1.281044000
7	-2.830687000	0.125855000	1.537068000	7	0.511204000	-1.961436000	-0.320159000
5	-2.173467000	-1.194738000	1.389665000	5	0.212907000	-1.146723000	-1.522767000
5	-1.489040000	0.446231000	2.079294000	5	1.207432000	-0.706963000	0.043956000
5	-0.899486000	-2.136477000	-0.415754000	5	-1.607946000	0.338596000	-2.018165000
7	-1.262970000	-1.611491000	-1.752524000	7	-2.871383000	0.003557000	-1.317914000
5	-2.478346000	-1.236784000	-0.991848000	5	-2.162551000	-1.292983000	-1.201092000
7	-2.231271000	-2.040658000	0.229684000	7	-1.067244000	-1.034163000	-2.166307000
5	0.505959000	1.236573000	1.001321000	5	0.434071000	1.258158000	1.200161000
7	0.260542000	2.038972000	-0.217377000	7	-0.661129000	0.998134000	2.165718000
5	-1.071131000	2.137199000	0.425666000	5	-0.120517000	-0.373898000	2.018019000
7	-0.708460000	1.611362000	1.764720000	7	1.143097000	-0.040009000	1.317827000
6	4.093557000	0.006923000	0.312940000	6	3.979645000	0.589770000	-0.000711000
1	3.821517000	0.004641000	1.364634000	16	4.497923000	-0.889490000	0.000516000
9	3.597563000	-1.083481000	-0.296407000	8	3.582911000	1.666437000	-0.001277000
9	5.412081000	0.000983000	0.149632000				
9	3.595455000	1.079039000	-0.302092000				
N ₂ O/B ₁₂ N ₁₂				AsH ₃ /B ₁₂ N ₁₂			
5	1.440184000	-0.674107000	-0.000077000	5	-0.399275000	1.680327000	-0.001002000
5	1.149622000	1.224387000	0.000126000	5	-1.430568000	-0.015430000	-0.000517000
7	1.450770000	0.304815000	1.122565000	7	-0.969428000	0.924068000	1.125409000
7	1.450732000	0.305057000	-1.122529000	7	-0.968992000	0.923113000	-1.127010000
7	0.756135000	-1.938380000	-0.000286000	7	0.856887000	2.396203000	-0.000996000
7	-1.469431000	-2.251021000	-0.000230000	7	2.887868000	1.426234000	-0.000136000
5	-0.377270000	-1.933429000	0.951687000	5	1.799782000	1.765970000	0.950400000
5	-0.377383000	-1.933219000	-0.952133000	5	1.800207000	1.765194000	-0.951438000
5	-2.460163000	-1.210726000	-0.000120000	5	3.129238000	0.009093000	0.000506000
5	-2.727551000	0.677864000	0.000115000	5	2.300623000	-1.708895000	0.000995000
7	-2.753472000	-0.288652000	1.123742000	7	2.861590000	-0.919242000	1.125331000
7	-2.753501000	-0.288382000	-1.123739000	7	2.862073000	-0.920115000	-1.123682000
7	0.161709000	2.267485000	0.000238000	7	-0.985502000	-1.434295000	0.000068000
7	-2.063490000	1.952789000	0.000245000	7	1.045627000	-2.403026000	0.000980000
5	-0.928146000	1.950085000	0.953770000	5	0.095276000	-1.756942000	0.943004000
5	-0.928201000	1.950269000	-0.953317000	5	0.095782000	-1.757713000	-0.942034000
5	0.292688000	0.141413000	1.958725000	5	0.083167000	0.414845000	1.942002000
7	-0.494068000	-1.103838000	2.120416000	7	1.434176000	1.014030000	2.118211000
5	-1.595718000	-0.125304000	1.959829000	5	1.802946000	-0.410805000	1.957557000
7	-0.808963000	1.121061000	2.121536000	7	0.456789000	-1.009751000	2.118189000
5	0.292624000	0.141821000	-1.958695000	5	0.083989000	0.413277000	-1.942751000
7	-0.494149000	-1.103372000	-2.120691000	7	1.435092000	1.012348000	-2.118831000
5	-1.595790000	-0.124861000	-1.959864000	5	1.803820000	-0.412343000	-1.956847000
7	-0.809014000	1.121534000	-2.121280000	7	0.457761000	-1.011443000	-2.117627000
7	4.295648000	0.020343000	-0.000041000	33	-3.702527000	0.001307000	-0.000040000
7	4.631719000	1.081422000	-0.000092000	1	-4.395973000	1.337982000	0.013407000
8	3.921393000	-1.103375000	0.000098000	1	-4.430431000	-0.661290000	1.140003000
				1	-4.432743000	-0.639576000	-1.150805000
CH ₃ Cl/B ₁₂ N ₁₂				COCl ₂ /B ₁₂ N ₁₂			
5	-1.418844000	-0.369262000	-0.000342000	5	0.715069000	-0.675903000	-0.009849000
5	-0.835447000	1.462379000	-0.000413000	5	-0.333498000	-1.105002000	-1.556771000
7	-1.268832000	0.602084000	-1.123791000	7	0.601347000	0.018949000	-1.323685000
7	-1.269325000	0.602361000	1.122943000	7	0.010074000	-1.930874000	-0.377655000
7	-0.905994000	-1.716282000	-0.000102000	7	0.632436000	-0.026513000	1.278672000
7	1.250054000	-2.351223000	0.000356000	7	-1.174744000	0.961360000	2.180646000
5	0.214722000	-1.876537000	-0.950617000	5	-0.105475000	1.252530000	1.194929000
5	0.214420000	-1.876352000	0.950851000	5	-0.607731000	-0.397464000	1.995351000
5	2.380392000	-1.465624000	0.000450000	5	-2.468783000	1.056468000	1.564348000
5	2.919414000	0.363840000	0.000372000	5	-3.485191000	0.614557000	0.012435000
7	2.805112000	-0.595652000	-1.123478000	7	-2.809916000	1.882448000	0.380855000

7	2.804718000	-0.595407000	1.124369000	7	-3.403883000	-0.069090000	1.325253000
7	0.291157000	2.356151000	-0.000349000	7	-1.629360000	-1.010287000	-2.176439000
7	2.447818000	1.722159000	0.000094000	7	-3.436924000	-0.023509000	-1.274470000
5	1.324145000	1.883675000	-0.953444000	5	-2.194804000	0.347281000	-1.994499000
5	1.323837000	1.883940000	0.953207000	5	-2.697680000	-1.307044000	-1.193328000
5	-0.146514000	0.271346000	-1.957594000	5	-0.117727000	1.253442000	-1.204631000
7	0.451664000	-1.074000000	-2.120476000	7	-0.239911000	2.077115000	0.023654000
5	1.683088000	-0.265997000	-1.959540000	5	-1.648916000	2.094772000	-0.440109000
7	1.086068000	1.081766000	-2.121586000	7	-1.440123000	1.556154000	-1.804793000
5	-0.147199000	0.271824000	1.957114000	5	-1.148672000	-2.142796000	0.441207000
7	0.450891000	-1.073476000	2.120565000	7	-1.362153000	-1.606068000	1.807333000
5	1.682410000	-0.265527000	1.959966000	5	-2.683915000	-1.308419000	1.207166000
7	1.085304000	1.082270000	2.121433000	7	-2.559112000	-2.127274000	-0.021651000
6	-4.379799000	1.112246000	-0.000091000	6	3.871675000	-0.279160000	-0.015532000
1	-3.894096000	1.496859000	-0.892708000	17	5.591277000	-0.549037000	0.023101000
17	-4.179392000	-0.668812000	0.000073000	17	3.446259000	1.406816000	-0.009922000
1	-5.443372000	1.329574000	-0.007421000	8	3.088043000	-1.154533000	-0.042017000
1	-3.906632000	1.496106000	0.899541000				
C ₂ H ₂ /B ₁₂ N ₁₂				C ₂ H ₄ /B ₁₂ N ₁₂			
5	0.874608000	1.607330000	-0.623372000	5	-0.817488000	-0.000381000	1.729990000
5	1.764341000	0.001676000	-0.070170000	5	-1.718750000	-0.000065000	0.034788000
7	1.415436000	0.491627000	-1.430700000	7	-1.393536000	-1.123622000	0.957270000
7	1.483410000	1.257077000	0.680263000	7	-1.393595000	1.123133000	0.957721000
7	-0.394648000	2.256802000	-0.817435000	7	0.455753000	-0.000484000	2.401906000
7	-2.404021000	1.331148000	-0.418808000	7	2.462702000	-0.000228000	1.388085000
5	-1.355123000	1.333655000	-1.467090000	5	1.385759000	-0.953008000	1.750548000
5	-1.297810000	1.980858000	0.324955000	5	1.385706000	0.952346000	1.750931000
5	-2.627576000	-0.001853000	0.069979000	5	2.680927000	0.000064000	-0.032602000
5	-1.773747000	-1.613766000	0.625459000	5	1.820523000	0.000383000	-1.734510000
7	-2.378728000	-1.256046000	-0.680218000	7	2.395243000	-1.123674000	-0.956559000
7	-2.311583000	-0.492380000	1.432877000	7	2.395181000	1.124163000	-0.956108000
7	1.506469000	-1.332832000	0.418560000	7	-1.460544000	0.000227000	-1.387647000
7	-0.503744000	-2.257752000	0.817835000	7	0.547621000	0.000481000	-2.400815000
5	0.400182000	-1.978038000	-0.323965000	5	-0.384095000	-0.950025000	-1.746450000
5	0.458938000	-1.332613000	1.464622000	5	-0.384145000	0.950679000	-1.746066000
5	0.347070000	-0.272068000	-2.008710000	5	-0.350878000	-1.955851000	0.430483000
7	-1.014270000	0.229594000	-2.321607000	7	1.007868000	-2.121303000	1.003531000
5	-1.358411000	-1.058216000	-1.673947000	5	1.351142000	-1.959751000	-0.429096000
7	-0.008537000	-1.670661000	-1.667187000	7	-0.006569000	-2.120728000	-1.002186000
5	0.464105000	1.058047000	1.670955000	5	-0.350977000	1.955622000	0.431273000
7	-0.887548000	1.671082000	1.666978000	7	1.007760000	2.120919000	1.004386000
5	-1.240738000	0.273311000	2.011239000	5	1.351041000	1.959975000	-0.428306000
7	0.118849000	-0.229057000	2.320684000	7	-0.006679000	2.121109000	-1.001333000
6	4.600083000	-0.597587000	-0.001101000	6	-4.496194000	-0.664060000	-0.006732000
6	4.598160000	0.600166000	-0.001817000	6	-4.496168000	0.664072000	-0.006718000
1	4.591836000	-1.662341000	0.004725000	1	-4.673915000	-1.233570000	0.898221000
1	4.591921000	1.665027000	0.004312000	1	-4.673862000	1.233571000	0.898248000
				1	-4.310135000	1.228487000	-0.914208000
				1	-4.310181000	-1.228463000	-0.914234000
H ₂ Se/B ₁₂ N ₁₂				H ₂ S/B ₁₂ N ₁₂			
5	-1.378923000	0.006060000	-0.004789000	5	-1.847173000	0.003696000	0.035001000
5	-0.375837000	1.678225000	0.240508000	5	-0.827931000	-1.658225000	-0.292386000
7	-0.948731000	1.090418000	-0.982298000	7	-1.386201000	-1.123688000	0.959824000
7	-0.954186000	0.766484000	1.244447000	7	-1.416625000	-0.708094000	-1.252778000
7	-0.986467000	-1.400695000	-0.206839000	7	-1.421914000	1.400891000	0.286846000
7	1.035323000	-2.377890000	-0.344827000	7	0.606953000	2.362089000	0.440663000
5	0.093777000	-1.597700000	-1.188339000	5	-0.329730000	1.551064000	1.261075000
5	0.090622000	-1.868792000	0.681049000	5	-0.352771000	1.897042000	-0.592518000

5	2.296874000	-1.702040000	-0.243807000	5	1.863433000	1.685613000	0.297358000
5	3.139514000	-0.009085000	0.003807000	5	2.696086000	0.000906000	-0.029091000
7	2.866446000	-0.764263000	-1.242347000	7	2.440727000	0.705502000	1.249972000
7	2.861633000	-1.087394000	0.983064000	7	2.411345000	1.119318000	-0.960381000
7	0.886179000	2.371916000	0.344644000	7	0.428778000	-2.354959000	-0.440290000
7	2.908246000	1.395114000	0.207110000	7	2.457176000	-1.393086000	-0.286857000
5	1.826153000	1.877038000	-0.687016000	5	1.382867000	-1.906505000	0.599540000
5	1.822230000	1.603517000	1.196360000	5	1.358462000	-1.556575000	-1.270643000
5	0.101654000	0.696977000	-1.867254000	5	-0.323848000	-0.769482000	1.845326000
7	0.464528000	-0.691408000	-2.241618000	7	0.049456000	0.600830000	2.272101000
5	1.814828000	-0.132987000	-1.995243000	5	1.394462000	0.048031000	1.988269000
7	1.457488000	1.303491000	-1.951074000	7	1.030935000	-1.384112000	1.889900000
5	0.094028000	0.137714000	1.984021000	5	-0.373466000	-0.054177000	-1.975368000
7	0.455350000	-1.300369000	1.951324000	7	-0.005774000	1.380175000	-1.889837000
5	1.806874000	-0.695591000	1.879923000	5	1.344064000	0.768154000	-1.859341000
7	1.448398000	0.694472000	2.244081000	7	0.975762000	-0.604409000	-2.275826000
34	-3.801067000	-0.010838000	-0.055981000	16	-4.043460000	0.023497000	0.097937000
1	-3.956585000	1.230933000	0.710819000	1	-4.220693000	-1.155434000	-0.521502000
1	-3.925539000	-0.828270000	1.156771000	1	-4.200553000	0.728585000	-1.034957000
PH ₃ /B ₁₂ N ₁₂				COF ₂ /B ₁₂ N ₁₂			
5	-0.826629000	1.677701000	-0.000592000	5	1.175739000	-0.627061000	0.024232000
5	-1.893553000	-0.014737000	0.000036000	5	0.149012000	-1.095553000	-1.525785000
7	-1.398986000	0.928048000	1.127214000	7	1.069272000	0.043700000	-1.304040000
7	-1.398983000	0.927152000	-1.127800000	7	0.488120000	-1.894894000	-0.327740000
7	0.429999000	2.395962000	-0.000900000	7	1.072684000	0.048694000	1.298296000
7	2.460832000	1.424355000	-0.000591000	7	-0.757064000	1.031045000	2.161254000
5	1.372533000	1.764932000	0.949826000	5	0.319037000	1.316609000	1.181344000
5	1.372453000	1.764209000	-0.951203000	5	-0.171364000	-0.323582000	2.008647000
5	2.699749000	0.006763000	-0.000039000	5	-2.045736000	1.098562000	1.529916000
5	1.869266000	-1.710367000	0.000630000	5	-3.040292000	0.614493000	-0.023571000
7	2.431602000	-0.921288000	1.124974000	7	-2.384676000	1.897372000	0.327261000
7	2.431539000	-0.922137000	-1.124321000	7	-2.964678000	-0.042689000	-1.303178000
7	-1.418156000	-1.436743000	0.000587000	7	-1.141008000	-1.029112000	-2.160811000
7	0.614603000	-2.403828000	0.000899000	7	-2.970232000	-0.047704000	-1.297352000
5	-0.336666000	-1.755550000	0.941318000	5	-1.724925000	0.324550000	-2.011409000
5	-0.336727000	-1.756213000	-0.939959000	5	-2.216499000	-1.320043000	-1.183343000
5	-0.346526000	0.416462000	1.939399000	5	0.332409000	1.271080000	-1.216407000
7	1.006189000	1.013545000	2.117514000	7	0.185712000	2.115746000	-0.006495000
5	1.372589000	-0.411511000	1.956465000	5	-1.217423000	2.107751000	-0.485448000
7	0.025761000	-1.008751000	2.116946000	7	-0.986891000	1.545653000	-1.837451000
5	-0.346612000	0.415002000	-1.939756000	5	-0.676153000	-2.105456000	0.483050000
7	1.006097000	1.011940000	-2.118328000	7	-0.909566000	-1.544679000	1.836165000
5	1.372486000	-0.412999000	-1.956159000	5	-2.228558000	-1.274946000	1.216864000
7	0.025667000	-1.010371000	-2.116197000	7	-2.081361000	-2.115922000	0.005471000
15	-3.971541000	0.003906000	0.000044000	6	4.187647000	-0.112085000	0.001766000
1	-4.580288000	1.267435000	-0.000439000	9	5.489110000	-0.053773000	-0.013839000
1	-4.610860000	-0.614560000	1.084905000	9	3.716888000	1.103907000	0.005855000
1	-4.610714000	-0.615107000	-1.084950000	8	3.550213000	-1.095149000	0.010831000
CH ₃ F/B ₁₂ N ₁₂				HCHO/B ₁₂ N ₁₂			
5	-1.700764000	-0.358081000	0.000606000	5	-1.925960000	-0.305421000	-0.000070000
5	-1.068560000	1.471167000	0.021721000	5	-0.662737000	-1.839096000	0.000276000
7	-1.514083000	0.632837000	-1.111293000	7	-1.325060000	-1.162189000	1.125044000
7	-1.508896000	0.605057000	1.135291000	7	-1.324898000	-1.162503000	-1.124767000
7	-1.163048000	-1.701948000	-0.017565000	7	-1.663799000	1.173562000	-0.000271000
7	0.989393000	-2.352570000	-0.030447000	7	0.229613000	2.396086000	-0.000370000
5	-0.047538000	-1.855610000	-0.969991000	5	-0.625688000	1.631466000	0.941025000
5	-0.043326000	-1.879110000	0.925594000	5	-0.625621000	1.631184000	-0.941616000
5	2.124108000	-1.474154000	-0.021855000	5	1.567554000	1.875473000	-0.000243000

5	2.676869000	0.351416000	-0.000531000	5	2.616564000	0.284235000	0.000052000
7	2.553219000	-0.592963000	-1.136092000	7	2.227675000	1.170635000	1.124670000
7	2.558350000	-0.620871000	1.111949000	7	2.227798000	1.170295000	-1.124880000
7	0.063312000	2.360993000	0.030249000	7	0.680563000	-2.381198000	0.000375000
7	2.216591000	1.713550000	0.017374000	7	2.565928000	-1.151225000	0.000273000
5	1.090457000	1.894014000	-0.930655000	5	1.530610000	-1.632044000	0.950665000
5	1.094832000	1.870441000	0.974804000	5	1.530679000	-1.632337000	-0.950060000
5	-0.395770000	0.305567000	-1.947719000	5	-0.351586000	-0.523089000	1.939053000
7	0.192909000	-1.041541000	-2.131967000	7	-0.169441000	0.941617000	2.115692000
5	1.430123000	-0.244684000	-1.964013000	5	1.244745000	0.525412000	1.956501000
7	0.843369000	1.109253000	-2.108226000	7	1.069203000	-0.933838000	2.118317000
5	-0.386904000	0.257315000	1.958418000	5	-0.351399000	-0.523689000	-1.938959000
7	0.202401000	-1.093969000	2.106385000	7	-0.169238000	0.940968000	-2.116026000
5	1.438972000	-0.293177000	1.953205000	5	1.244936000	0.524805000	-1.956598000
7	0.852941000	1.056794000	2.133598000	7	1.069399000	-0.934500000	-2.117977000
6	-4.528058000	0.497077000	-0.001615000	6	-4.338756000	0.382012000	0.000061000
1	-4.267022000	1.063080000	-0.893980000	1	-5.408928000	0.163378000	0.000089000
9	-3.752314000	-0.670964000	0.002755000	1	-3.955712000	1.407335000	0.000178000
1	-5.571454000	0.190819000	-0.016467000	8	-3.560938000	-0.552654000	-0.000164000
1	-4.290062000	1.054439000	0.902613000				
(CH ₃) ₂ O/B ₁₂ N ₁₂				CH ₃ NH ₂ /B ₁₂ N ₁₂			
5	1.724472000	-0.015098000	-0.221397000	5	0.690818000	-1.043045000	-1.437748000
5	0.703362000	-1.443036000	0.750307000	5	1.914764000	-0.390939000	0.024956000
7	1.163192000	-1.392108000	-0.645266000	7	1.152916000	-1.732799000	-0.226385000
7	1.341217000	-0.229101000	1.278289000	7	1.481435000	0.193190000	-1.360907000
7	1.181903000	1.208922000	-0.899281000	7	-0.606039000	-1.193691000	-2.068228000
7	-0.877982000	2.058220000	-1.227308000	7	-2.535596000	-0.378962000	-1.241428000
5	0.023975000	1.009559000	-1.776692000	5	-1.624888000	-1.537192000	-1.052461000
5	0.164716000	1.974310000	-0.172058000	5	-1.349360000	0.083372000	-2.005940000
5	-2.102161000	1.475417000	-0.763775000	5	-2.657359000	0.363089000	-0.016425000
5	-2.868971000	0.013008000	0.190796000	5	-1.702041000	1.076958000	1.472292000
7	-2.721758000	0.225258000	-1.269153000	7	-2.482511000	-0.179868000	1.352391000
7	-2.547316000	1.385854000	0.650063000	7	-2.156052000	1.738378000	0.223304000
7	-0.521104000	-2.050325000	1.226479000	7	1.521937000	0.400620000	1.254219000
7	-2.581115000	-1.203908000	0.900320000	7	-0.411489000	1.214651000	2.079119000
5	-1.556677000	-1.993839000	0.170832000	5	0.342590000	-0.064488000	1.990863000
5	-1.410825000	-1.013719000	1.793809000	5	0.614157000	1.533615000	1.050842000
5	0.033289000	-1.365751000	-1.511961000	5	0.035827000	-1.994925000	0.613200000
7	-0.404109000	-0.233140000	-2.363669000	7	-1.374061000	-2.221531000	0.184406000
5	-1.711209000	-0.649286000	-1.806099000	5	-1.597130000	-1.315869000	1.333102000
7	-1.308260000	-1.957458000	-1.242279000	7	-0.244749000	-1.377869000	1.934712000
5	0.332657000	0.631819000	1.797265000	5	0.597044000	1.306213000	-1.330087000
7	-0.076100000	1.949031000	1.247299000	7	-0.759723000	1.390892000	-1.941860000
5	-1.409483000	1.368195000	1.532257000	5	-1.029947000	2.018710000	-0.629465000
7	-0.981466000	0.227866000	2.373069000	7	0.369130000	2.227436000	-0.187465000
8	3.323950000	-0.004644000	-0.366830000	7	3.505528000	-0.655753000	0.028790000
6	3.923779000	1.206049000	0.136716000	1	3.716649000	-1.262453000	-0.762835000
1	3.788257000	1.243793000	1.219780000	1	3.729204000	-1.178596000	0.875160000
1	4.979126000	1.190803000	-0.129290000	6	4.293917000	0.597194000	-0.037986000
1	3.410839000	2.028731000	-0.350777000	1	4.006643000	1.117798000	-0.949569000
6	3.993973000	-1.190718000	0.105859000	1	4.024602000	1.203267000	0.824481000
1	3.895259000	-1.246447000	1.191502000	1	5.361939000	0.386459000	-0.039642000
1	3.505104000	-2.032387000	-0.373659000				
1	5.037865000	-1.121011000	-0.194721000				

Table S4. Cartesian coordinates for the gas-adsorbed Al₁₂N₁₂ nanocages

SiH ₄ /Al ₁₂ N ₁₂				H ₂ /Al ₁₂ N ₁₂			
13	-0.467368000	-2.466762000	0.864677000	13	2.761350000	-0.050911000	-0.060821000
13	1.406856000	-2.459963000	-0.754816000	13	1.581418000	1.019090000	-1.967309000
7	1.364898000	-2.585577000	1.087322000	7	2.348376000	1.716321000	-0.439279000
7	-0.414250000	-2.688602000	-0.970501000	7	2.271937000	-0.677230000	-1.734397000
7	-1.562781000	-1.380094000	1.755029000	7	2.374969000	-0.879180000	1.478664000
7	-1.643350000	1.343489000	1.693233000	7	-0.048580000	-1.415372000	2.606000000
13	-0.659547000	0.027535000	2.532355000	13	1.119841000	0.012614000	2.497536000
13	-2.347431000	-0.063665000	0.706651000	13	1.052690000	-2.157350000	1.320151000
13	-0.610451000	2.450294000	0.754259000	13	-1.672506000	-1.024803000	1.979593000
13	1.264097000	2.476369000	-0.865420000	13	-2.805924000	0.052972000	0.059580000
7	1.212563000	2.684182000	0.968972000	7	-2.351972000	0.676974000	1.738486000
7	-0.566266000	2.590895000	-1.089460000	7	-2.427271000	-1.715256000	0.440355000
7	2.435572000	-1.342783000	-1.694075000	7	-0.039015000	1.414185000	-2.604021000
7	2.356453000	1.378962000	-1.754736000	7	-2.463063000	0.880172000	-1.484388000
13	3.076294000	0.061233000	-0.676976000	13	-1.141170000	2.161426000	-1.323641000
13	1.459126000	-0.027583000	-2.548705000	13	-1.206332000	-0.013686000	-2.503246000
13	2.048298000	-1.147708000	1.893365000	13	1.125732000	2.406361000	0.661095000
7	1.091560000	0.085027000	2.879836000	7	0.651253000	1.724700000	2.312384000
13	1.977002000	1.325360000	1.836332000	13	-1.075832000	1.924371000	1.688603000
7	3.156553000	0.104440000	1.104825000	7	-0.593226000	2.908673000	0.201235000
13	-1.175919000	-1.321000000	-1.826369000	13	0.992738000	-1.919045000	-1.684093000
7	-2.357625000	-0.103063000	-1.097116000	7	0.507048000	-2.911831000	-0.202347000
13	-1.246299000	1.145059000	-1.883877000	13	-1.210490000	-2.412637000	-0.664395000
7	-0.292496000	-0.084699000	-2.879481000	7	-0.735496000	-1.723567000	-2.311440000
14	-5.274642000	0.000532000	-0.041343000	1	4.874669000	0.309110000	-0.259444000
1	-4.248462000	-0.116263000	1.065198000	1	4.880921000	-0.278478000	0.210964000
1	-5.200961000	-1.203533000	-0.878881000				
1	-6.543949000	0.045731000	0.715752000				
1	-5.048020000	1.262188000	-0.759382000				
Cl ₂ /Al ₁₂ N ₁₂				F ₂ /Al ₁₂ N ₁₂			
13	2.056426000	-0.527730000	-0.190532000	13	2.409722000	0.039441000	-0.020630000
13	1.023723000	1.070470000	-1.839145000	13	1.240023000	1.349417000	-1.773518000
7	1.898025000	1.367651000	-0.227182000	7	1.957320000	1.832472000	-0.139889000
7	1.423544000	-0.719318000	-1.915939000	7	1.977958000	-0.342533000	-1.778909000
7	1.519967000	-1.516966000	1.195006000	7	2.051275000	-1.021053000	1.372195000
7	-0.937818000	-1.858908000	2.312474000	7	-0.365380000	-1.792636000	2.366774000
13	0.450251000	-0.644287000	2.414989000	13	0.756643000	-0.329237000	2.491947000
13	0.010990000	-2.523448000	0.871004000	13	0.773902000	-2.302435000	1.003578000
13	-2.479967000	-1.105966000	1.828338000	13	-1.993766000	-1.362165000	1.778659000
13	-3.441666000	0.472215000	0.179295000	13	-3.136434000	-0.044419000	0.020629000
7	-2.872270000	0.697645000	1.922858000	7	-2.726031000	0.334527000	1.782148000
7	-3.355249000	-1.372065000	0.222813000	7	-2.705927000	-1.837060000	0.140349000
7	-0.515664000	1.835668000	-2.303160000	7	-0.386298000	1.785592000	-2.366246000
7	-2.981829000	1.504481000	-1.202623000	7	-2.802679000	1.015489000	-1.375907000
13	-1.467587000	2.504955000	-0.868813000	13	-1.525319000	2.299160000	-1.005598000
13	-1.903428000	0.618840000	-2.413771000	13	-1.507367000	0.322487000	-2.496671000
13	0.827777000	2.027936000	1.052940000	13	0.704261000	2.315092000	1.034838000
7	0.270575000	1.128400000	2.557950000	7	0.234088000	1.376504000	2.555443000
13	-1.410898000	1.710616000	2.052742000	13	-1.491380000	1.613695000	1.939718000
7	-0.785769000	2.858977000	0.742556000	7	-1.024055000	2.824746000	0.624452000
13	-0.040699000	-1.735778000	-2.038186000	13	0.741305000	-1.617949000	-1.935396000
7	-0.668259000	-2.887534000	-0.739287000	7	0.271976000	-2.833500000	-0.624891000
13	-2.283851000	-2.045066000	-1.035989000	13	-1.455302000	-2.323825000	-1.036284000
7	-1.716738000	-1.148427000	-2.550287000	7	-0.984228000	-1.382328000	-2.554765000
17	4.177128000	0.602684000	-0.072671000	9	4.558957000	0.586440000	-0.006495000

17	6.035607000	-0.421687000	0.056578000	9	5.419057000	-0.496660000	0.004071000
CF ₄ /Al ₁₂ N ₁₂				CH ₄ /Al ₁₂ N ₁₂			
13	-0.316783000	-1.851142000	1.660088000	13	0.888869000	2.463769000	0.536886000
13	1.598119000	-2.645713000	0.305736000	13	-1.333279000	2.466220000	-0.556570000
7	1.479026000	-2.053881000	2.051654000	7	-0.824194000	2.640531000	1.210698000
7	-0.228581000	-2.760767000	0.053570000	7	0.378341000	2.635541000	-1.230931000
7	-1.304173000	-0.404272000	1.986805000	7	2.150444000	1.367078000	1.158439000
7	-1.057294000	2.082300000	0.903096000	7	2.151161000	-1.357270000	1.168215000
13	-0.267401000	1.099362000	2.251710000	13	1.440724000	0.008374000	2.187352000
13	-1.863120000	0.477751000	0.455788000	13	2.589616000	0.000757000	-0.016836000
13	0.130300000	2.639646000	-0.303683000	13	0.890213000	-2.459076000	0.554513000
13	2.046108000	1.857833000	-1.664826000	13	-1.331960000	-2.470965000	-0.538850000
7	1.958812000	2.757779000	-0.054048000	7	-0.822741000	-2.632139000	1.229600000
7	0.250945000	2.055112000	-2.053381000	7	0.379777000	-2.643907000	-1.212023000
7	2.783225000	-2.079920000	-0.903784000	7	-2.589800000	1.356577000	-1.170336000
7	3.030392000	0.404621000	-1.990495000	7	-2.589053000	-1.366367000	-1.160546000
13	3.552370000	-0.463476000	-0.444860000	13	-2.985311000	-0.000711000	0.019618000
13	1.997924000	-1.103741000	-2.262405000	13	-1.888610000	-0.008411000	-2.200343000
13	2.300953000	-0.490577000	2.306198000	13	-1.315423000	1.245193000	2.208209000
7	1.465995000	1.113657000	2.680508000	7	-0.167516000	0.010693000	2.963211000
13	2.527001000	1.767169000	1.316955000	13	-1.314664000	-1.229866000	-2.217036000
7	3.575320000	0.250383000	1.190715000	7	-2.612876000	0.005650000	1.765037000
13	-0.795349000	-1.760680000	-1.311644000	13	0.869864000	1.227359000	-2.211341000
7	-1.845816000	-0.248421000	-1.185385000	7	2.166076000	-0.005582000	-1.757545000
13	-0.571329000	0.489880000	-2.298969000	13	0.870496000	-1.242456000	-2.202395000
7	0.264425000	-1.113974000	-2.681196000	7	-0.277349000	-0.010611000	-2.965337000
6	-4.947008000	-0.025303000	-0.025849000	6	5.257145000	-0.000421000	0.003671000
9	-4.579869000	-1.276134000	0.041389000	1	4.914870000	0.902077000	0.518168000
9	-5.002841000	0.390017000	-1.257350000	1	4.936943000	-0.006076000	-1.041570000
9	-4.025347000	0.727526000	0.644928000	1	6.346268000	0.000766000	0.019966000
9	-6.095077000	0.149861000	0.575205000	1	4.916194000	-0.898037000	0.527401000
CF ₂ Cl ₂ /Al ₁₂ N ₁₂				N ₂ /Al ₁₂ N ₁₂			
13	0.432419000	1.211841000	-1.858754000	13	2.520402000	0.001602000	0.048476000
13	0.136859000	2.387211000	0.289889000	13	1.372630000	0.006493000	-2.160484000
7	1.468474000	1.273198000	-0.333345000	7	2.077013000	1.366530000	-1.131582000
7	-0.696091000	2.585173000	-1.349093000	7	2.078607000	-1.357963000	-1.138476000
7	-0.058943000	-0.263638000	-2.734577000	7	2.058208000	-0.003086000	1.781919000
7	-1.682222000	-2.265522000	-1.858741000	7	-0.400008000	-0.007562000	2.963223000
13	0.092159000	-1.774050000	-1.678678000	13	0.756259000	1.228180000	2.218916000
13	-1.873055000	-0.588574000	-2.609274000	13	0.757795000	-1.238174000	2.212632000
13	-2.510571000	-2.413079000	-0.285250000	13	-2.002462000	-0.006553000	2.181114000
13	-2.806391000	-1.234349000	1.870992000	13	-3.074524000	-0.001509000	-0.050707000
7	-1.677731000	-2.600777000	1.352731000	7	-2.692989000	1.357344000	1.141981000
7	-3.842957000	-1.295625000	0.341463000	7	-2.691386000	-1.365936000	1.135144000
7	-0.691979000	2.252455000	1.865016000	7	-0.223769000	0.007531000	-2.960878000
7	-2.314062000	0.247218000	2.734640000	7	-2.683613000	0.003106000	-1.792132000
13	-0.497298000	0.569871000	2.606805000	13	-1.380857000	1.242384000	-2.221244000
13	-2.464696000	1.763449000	1.690184000	13	-1.379338000	-1.232415000	-2.227532000
13	1.561615000	-0.291998000	0.541115000	13	0.805405000	2.459810000	-0.526961000
7	1.075786000	-1.921420000	-0.200980000	7	0.274761000	2.637386000	1.234668000
13	0.034217000	-2.092355000	1.311359000	13	-1.429026000	2.466265000	0.541585000
7	0.750809000	-0.625574000	2.172818000	7	-0.900375000	2.638630000	-1.220013000
13	-2.408539000	2.088655000	-1.314077000	13	0.808346000	-2.455849000	-0.539396000
7	-3.119490000	0.610638000	-2.166580000	7	0.277927000	-2.642999000	1.221336000
13	-3.884704000	0.266678000	-0.519898000	13	-1.426090000	-2.470257000	0.529154000
7	-3.445567000	1.908560000	0.205326000	7	-0.897246000	-2.633062000	-1.233293000
6	4.619740000	-0.067604000	-0.101457000	7	4.726831000	0.000769000	0.012356000
9	3.686441000	-0.423915000	0.853855000	7	5.814463000	-0.000647000	-0.024566000

9	4.066294000	-0.326274000	-1.268655000			
17	6.016751000	-1.089035000	0.145257000			
17	4.959047000	1.630894000	0.064381000			
CHF ₃ /Al ₁₂ N ₁₂				OCS/Al ₁₂ N ₁₂		
13	-0.075989000	-2.637740000	-0.043842000	13	0.326800000	-0.804106000 2.454381000
13	1.836748000	-2.035253000	-1.499221000	13	-1.564067000	0.796801000 2.470673000
7	1.753742000	-2.773747000	0.190593000	7	-1.499815000	-1.041675000 2.631624000
7	0.031171000	-2.228708000	-1.844514000	7	0.259991000	1.034261000 2.644622000
7	-1.236547000	-1.940664000	1.111304000	7	1.402858000	-1.704130000 1.356931000
7	-1.415775000	0.640711000	1.957181000	7	1.404385000	-1.693758000 -1.367198000
13	-0.405370000	-0.851103000	2.346266000	13	0.463124000	-2.510125000 -0.008648000
13	-2.051858000	-0.375648000	0.543085000	13	2.151761000	-0.675652000 -0.000923000
13	-0.403943000	2.026615000	1.486566000	13	0.329777000	-0.785531000 -2.459337000
13	1.507857000	2.645995000	0.037354000	13	-1.561268000	0.815272000 -2.465901000
7	1.402372000	2.226525000	1.831834000	7	-1.496615000	-1.021927000 -2.640369000
7	-0.320076000	2.776227000	-0.202187000	7	0.263065000	1.054166000 -2.635989000
7	2.844152000	-0.640063000	-1.975141000	7	-2.634719000	1.704702000 1.367051000
7	2.663282000	1.941501000	-1.127499000	7	-2.633048000	1.714859000 -1.356555000
13	3.406804000	0.359737000	-0.525597000	13	-3.304123000	0.655354000 0.000903000
13	1.840042000	0.857627000	-2.376019000	13	-1.704518000	2.544408000 0.008899000
13	2.361477000	-1.669477000	1.454051000	13	-2.216672000	-1.880211000 1.229507000
7	1.332787000	-0.864831000	2.758722000	7	-1.284459000	-2.880318000 -0.011106000
13	2.196174000	0.677107000	2.223870000	13	-2.215018000	-1.870990000 -1.245395000
7	3.439961000	-0.194983000	1.169643000	7	-3.368076000	-1.127664000 -0.005894000
13	-0.759069000	-0.675951000	-2.221929000	13	0.973138000	1.872991000 1.240820000
7	-2.017903000	0.192960000	-1.178654000	7	2.127418000	1.130306000 0.005744000
13	-0.925835000	1.662551000	-1.455345000	13	0.974786000	1.882270000 -1.225147000
7	0.099335000	0.864369000	-2.768097000	7	0.044584000	2.892782000 0.011080000
6	-4.899870000	0.021825000	-0.315354000	6	4.985849000	0.511431000 0.000645000
9	-4.081492000	-0.548839000	0.674999000	8	5.251750000	1.615557000 0.001398000
9	-6.004759000	-0.689719000	-0.312276000	16	4.717097000	-1.059408000 -0.000780000
9	-5.152309000	1.247878000	0.090219000			
1	-4.340755000	-0.007863000	-1.246736000			
N ₂ O/Al ₁₂ N ₁₂				AsH ₃ /Al ₁₂ N ₁₂		
13	0.466205000	-0.833162000	2.451072000	13	0.534366000	0.383159000 2.452859000
13	-1.381647000	0.817054000	2.473040000	13	-0.539106000	-1.849712000 2.469235000
7	-1.365711000	-1.022556000	2.631043000	7	1.224002000	-1.326087000 2.635393000
7	0.448204000	1.006668000	2.645607000	7	-1.227787000	-0.145083000 2.643876000
7	1.518901000	-1.754678000	1.351387000	7	1.140741000	1.656080000 1.364722000
7	1.517515000	-1.738612000	-1.373107000	7	1.140741000	1.656080000 -1.364722000
13	0.559805000	-2.535280000	-0.014961000	13	2.147867000	0.939488000 0.000000000
13	2.299454000	-0.750915000	-0.005516000	13	-0.040454000	2.159878000 0.000000000
13	0.463822000	-0.804074000	-2.460675000	13	0.534366000	0.383159000 -2.452859000
13	-1.383866000	0.846434000	-2.462934000	13	-0.539106000	-1.849712000 -2.469235000
7	-1.368073000	-0.991284000	-2.641880000	7	1.224002000	-1.326087000 -2.635393000
7	0.445878000	1.037948000	-2.634248000	7	-1.227787000	-0.145083000 -2.643876000
7	-2.430682000	1.754035000	1.372867000	7	-1.143334000	-3.114517000 1.362125000
7	-2.432141000	1.770151000	-1.350811000	7	-1.143334000	-3.114517000 -1.362125000
13	-3.128275000	0.724559000	0.005293000	13	0.044905000	-3.499039000 0.000000000
13	-1.480006000	2.571035000	0.015288000	13	-2.183156000	-2.420829000 0.000000000
13	-2.103588000	-1.839786000	1.227095000	13	2.219707000	-1.810826000 1.236913000
7	-1.197736000	-2.859796000	-0.016478000	7	2.955775000	-0.655158000 0.000000000
13	-2.104598000	-1.825301000	-1.247158000	13	2.219707000	-1.810826000 -1.236913000
7	-3.237944000	-1.056189000	-0.004990000	7	1.788018000	-3.116198000 0.000000000
13	1.181746000	1.827070000	1.241493000	13	-2.206253000	0.339633000 1.230955000
7	2.320124000	1.061511000	0.005172000	7	-1.770035000	1.636819000 0.000000000
13	1.180977000	1.841864000	-1.221397000	13	-2.206253000	0.339633000 -1.230955000
7	0.277330000	2.874187000	0.016647000	7	-2.961095000	-0.817582000 0.000000000

7	4.997346000	0.030055000	-0.000237000	33	0.002071000	4.792483000	0.000000000
7	5.612279000	0.946647000	0.005636000	1	-1.279141000	5.584131000	0.000000000
8	4.356573000	-0.990008000	-0.006823000	1	0.692887000	5.495588000	-1.138223000
				1	0.692887000	5.495588000	1.138223000
CH ₃ Cl/Al ₁₂ N ₁₂				COCl ₂ /Al ₁₂ N ₁₂			
13	-0.650045000	0.411617000	-2.448268000	13	1.790527000	-0.720706000	0.010233000
13	1.702401000	-0.368514000	-2.469681000	13	0.383338000	-1.242794000	2.008081000
7	0.099545000	-1.265717000	-2.650191000	7	0.877794000	-2.249970000	0.549615000
7	0.957471000	1.315447000	-2.621456000	7	1.487511000	0.182239000	1.625066000
7	-1.990808000	0.846746000	-1.354309000	7	1.488688000	0.070004000	-1.586918000
7	-1.991211000	0.823688000	1.368967000	7	-0.756622000	1.124979000	-2.723254000
13	-2.317761000	-0.413732000	-0.003205000	13	0.010619000	-0.545589000	-2.495752000
13	-1.390461000	1.919356000	0.016553000	13	0.548550000	1.650055000	-1.523954000
13	-0.650167000	0.369303000	2.454542000	13	-2.397025000	1.226841000	-2.034635000
13	1.702200000	-0.411526000	2.463018000	13	-3.686392000	0.651312000	-0.001448000
7	0.099325000	-1.311405000	2.628769000	7	-3.485907000	-0.208987000	-1.624032000
7	0.957630000	1.269665000	2.643463000	7	-2.878677000	2.220932000	-0.552201000
7	3.035554000	-0.817212000	-1.369323000	7	-1.254531000	-1.149432000	2.720049000
7	3.035437000	-0.840392000	1.354798000	7	-3.508779000	-0.101860000	1.606376000
13	2.481927000	-1.950607000	-0.016949000	13	-2.564115000	-1.691407000	1.537153000
13	3.267889000	0.397140000	0.003198000	13	-2.019986000	0.516384000	2.510671000
13	-0.253162000	-2.317593000	-1.251119000	13	-0.524365000	-2.682377000	-0.456460000
7	-1.591720000	-2.058306000	-0.016931000	7	-0.882832000	-2.053776000	-2.159250000
13	-0.253180000	-2.340396000	1.212562000	13	-2.571868000	-1.737931000	-1.484144000
7	0.991632000	-2.927309000	-0.024719000	7	-2.297827000	-2.682885000	0.078662000
13	1.321208000	2.353458000	-1.217664000	13	0.557804000	1.691970000	1.478645000
7	0.082494000	2.928142000	0.025315000	7	0.293813000	2.664354000	-0.075065000
13	1.321589000	2.330819000	1.257378000	13	-1.476886000	2.669241000	0.459049000
7	2.669511000	2.078795000	0.017273000	7	-1.132898000	2.023027000	2.154096000
6	-5.084708000	1.122608000	0.010107000	6	4.653334000	-0.209597000	0.005424000
1	-4.628584000	1.518071000	0.913846000	17	4.385461000	1.475794000	-0.044877000
17	-4.719037000	-0.648914000	-0.006816000	17	6.296499000	-0.691026000	0.017078000
1	-6.165598000	1.216489000	0.011626000	8	3.773239000	-1.019857000	0.031413000
1	-4.629661000	1.535125000	-0.886574000				
C ₂ H ₂ /Al ₁₂ N ₁₂				C ₂ H ₄ /Al ₁₂ N ₁₂			
13	2.592980000	0.089310000	-0.004118000	13	2.555245000	0.001142000	-0.013059000
13	1.275306000	2.220778000	-0.019738000	13	1.303241000	0.007044000	-2.182175000
7	2.044044000	1.258694000	1.348242000	7	2.034816000	1.368479000	-1.179756000
7	2.040441000	1.236451000	-1.373803000	7	2.036135000	-1.359724000	-1.187902000
7	2.157739000	-1.667338000	0.010041000	7	2.069123000	-0.004317000	1.726771000
7	-0.243570000	-2.961767000	0.023795000	7	-0.364783000	-0.009059000	2.962651000
13	0.878085000	-2.147029000	1.247634000	13	0.777823000	1.224013000	2.190799000
13	0.874192000	-2.166018000	-1.215910000	13	0.779111000	-1.236712000	2.183900000
13	-1.881276000	-2.257647000	0.020218000	13	-1.981984000	-0.007292000	2.213829000
13	-3.058558000	-0.080429000	0.004181000	13	-3.098996000	-0.001093000	0.004528000
7	-2.617030000	-1.238611000	1.375238000	7	-2.693270000	1.357552000	1.189701000
7	-2.620282000	-1.260410000	-1.349144000	7	-2.692129000	-1.366539000	1.181547000
7	-0.351538000	2.958605000	-0.023577000	7	-0.306688000	0.008819000	-2.958110000
7	-2.754441000	1.677767000	-0.010309000	7	-2.745738000	0.004213000	-1.744882000
13	-1.469442000	2.179114000	1.221273000	13	-1.449905000	1.242974000	-2.197665000
13	-1.472595000	2.159769000	-1.253076000	13	-1.448789000	-1.230644000	-2.204843000
13	0.804041000	0.605753000	2.448138000	13	0.772094000	2.455092000	-0.547986000
7	0.354950000	-1.177051000	2.650900000	7	0.276900000	2.639119000	1.223864000
13	-1.379495000	-0.567558000	2.474705000	13	-1.440428000	2.466875000	0.565698000
7	-0.934882000	1.218145000	2.625981000	7	-0.948220000	2.638518000	-1.206278000
13	0.797737000	0.566584000	-2.460395000	13	0.774435000	-2.451268000	-0.562595000
7	0.347832000	-1.219148000	-2.633565000	7	0.279387000	-2.646246000	1.208241000
13	-1.385981000	-0.606721000	-2.462623000	13	-1.438045000	-2.470773000	0.551151000

7	-0.941727000	1.176293000	-2.643574000	7	-0.945844000	-2.631619000	-1.221778000
6	4.946869000	0.604627000	0.000528000	6	4.915209000	0.670296000	0.002384000
6	4.931853000	-0.598596000	-0.001476000	6	4.915471000	-0.668548000	-0.002822000
1	4.886532000	-1.665349000	-0.002585000	1	4.817102000	-1.228690000	0.922392000
1	4.995455000	1.670980000	0.002950000	1	4.816626000	1.223197000	0.931940000
				1	5.017653000	-1.235760000	-0.920244000
				1	5.017268000	1.244734000	-0.910496000
H ₂ Se/Al ₁₂ N ₁₂				H ₂ S/Al ₁₂ N ₁₂			
13	2.165713000	-0.013542000	0.013598000	13	2.506625000	-0.128768000	-0.005479000
13	0.927571000	-0.060588000	-2.164150000	13	1.265327000	0.150966000	-2.164049000
7	1.661396000	1.326353000	-1.198609000	7	2.056543000	1.376685000	-1.036917000
7	1.649193000	-1.401781000	-1.130623000	7	1.934633000	-1.335632000	-1.311177000
7	1.663152000	0.039139000	1.748354000	7	2.010378000	-0.270953000	1.726146000
7	-0.780133000	0.076245000	2.961623000	7	-0.429279000	-0.295710000	2.947775000
13	0.372465000	1.283573000	2.164509000	13	0.766699000	0.957825000	2.301123000
13	0.366921000	-1.177587000	2.228306000	13	0.669779000	-1.490001000	2.057546000
13	-2.390828000	0.061781000	2.199206000	13	-2.040440000	-0.153145000	2.199671000
13	-3.490257000	0.008891000	-0.018025000	13	-3.144117000	0.114950000	0.000006000
7	-3.088949000	1.399790000	1.130912000	7	-2.687482000	1.334211000	1.311854000
7	-3.098240000	-1.323624000	1.200671000	7	-2.801955000	-1.373860000	1.039279000
7	-0.674736000	-0.075066000	-2.955836000	7	-0.337544000	0.296525000	-2.940779000
7	-3.123622000	-0.037139000	-1.764021000	7	-2.782397000	0.275480000	-1.740352000
13	-1.819507000	1.183753000	-2.240729000	13	-1.433979000	1.497189000	-2.067964000
13	-1.826627000	-1.289378000	-2.176728000	13	-1.533730000	-0.962669000	-2.314138000
13	0.395332000	2.432754000	-0.609104000	13	0.830554000	2.444465000	-0.307041000
7	-0.114468000	2.671871000	1.152637000	7	0.333795000	2.480062000	1.474367000
13	-1.826721000	2.486001000	0.485412000	13	-1.385813000	2.444681000	0.800349000
7	-1.319481000	2.605609000	-1.286354000	7	-0.876978000	2.767004000	-0.945566000
13	0.380012000	-2.471034000	-0.483244000	13	0.628417000	-2.431325000	-0.796500000
7	-0.131730000	-2.611377000	1.288353000	7	0.114113000	-2.772720000	0.946901000
13	-1.842425000	-2.449424000	0.612397000	13	-1.589747000	-2.462398000	0.307108000
7	-1.336800000	-2.663742000	-1.150862000	7	-1.095406000	-2.472502000	-1.472189000
34	4.786564000	-0.053014000	0.014742000	16	4.989265000	-0.092500000	-0.002704000
1	4.903818000	1.247114000	0.687669000	1	5.051977000	0.872345000	0.931289000
1	4.862505000	0.573825000	-1.311463000	1	5.036323000	0.784510000	-1.021621000
PH ₃ /Al ₁₂ N ₁₂				COF ₂ /Al ₁₂ N ₁₂			
13	0.717260000	-2.455746000	-0.537465000	13	-2.117388000	-0.714947000	-0.016898000
13	-1.528605000	-2.464906000	0.508772000	13	-0.729357000	-1.160866000	-2.042976000
7	-0.984700000	-2.623921000	-1.248829000	7	-1.213514000	-2.222206000	-0.617713000
7	0.166203000	-2.655001000	1.216786000	7	-1.834553000	0.247769000	-1.600002000
7	2.005256000	-1.373185000	-1.121392000	7	-1.822204000	0.026790000	1.603507000
7	2.022426000	1.358151000	-1.103461000	7	0.430453000	1.044852000	2.761252000
13	1.309494000	0.003502000	-2.126339000	13	-0.335739000	-0.616904000	2.482319000
13	2.508347000	-0.019084000	0.075727000	13	-0.882244000	1.610292000	1.588779000
13	0.747667000	2.448295000	-0.504829000	13	2.067551000	1.173903000	2.068306000
13	-1.497939000	2.472019000	0.541717000	13	3.349199000	0.668815000	0.011496000
7	-0.951913000	2.647558000	-1.213665000	7	3.156300000	-0.246380000	1.604676000
7	0.199212000	2.631250000	1.251987000	7	2.543160000	2.218029000	0.618653000
7	-2.794255000	-1.354592000	1.105361000	7	0.904753000	-1.041253000	-2.757911000
7	-2.777206000	1.369572000	1.123632000	7	3.163333000	-0.029324000	-1.620359000
13	-3.155329000	0.017752000	-0.078408000	13	2.221813000	-1.621527000	-1.601426000
13	-2.104701000	-0.003756000	2.162888000	13	1.669888000	0.617815000	-2.496256000
13	-1.447521000	-1.215391000	-2.240560000	13	0.195093000	-2.685648000	0.366688000
7	-0.275116000	0.018967000	-2.954139000	7	0.557407000	-2.111226000	2.087052000
13	-1.431916000	1.258211000	-2.224124000	13	2.244049000	-1.770698000	1.416717000
7	-2.750330000	0.026892000	-1.816526000	7	1.964786000	-2.662952000	-0.176373000
13	0.648092000	-1.252081000	2.210987000	13	-0.905187000	1.754357000	-1.408733000
7	1.957778000	-0.026743000	1.798265000	7	-0.629869000	2.670823000	0.174858000

13	0.663355000	1.209095000	2.227099000	13	1.135611000	2.697720000	-0.369927000
7	-0.511044000	-0.019154000	2.960125000	7	0.781220000	2.108814000	-2.083938000
15	5.016795000	-0.000696000	-0.002563000	6	-4.887426000	-0.063663000	-0.002139000
1	5.746679000	-1.050779000	0.580058000	9	-4.564660000	1.176537000	0.077429000
1	5.701418000	1.092292000	0.555489000	9	-6.165040000	-0.204592000	-0.024336000
1	5.589148000	-0.002472000	-1.285173000	8	-4.123724000	-0.971467000	-0.049508000
CH ₃ F/Al ₁₂ N ₁₂				HCHO/Al ₁₂ N ₁₂			
13	-0.572049000	-2.054025000	-1.564512000	13	-2.550001000	-0.465745000	0.079670000
13	1.444116000	-0.874014000	-2.390459000	13	-1.492037000	0.704637000	-1.879964000
7	1.233816000	-2.444260000	-1.442734000	7	-1.946600000	-1.049450000	-1.591486000
7	-0.348164000	-0.693916000	-2.799460000	7	-2.315605000	1.366348000	-0.365523000
7	-1.747343000	-2.069877000	-0.230569000	7	-1.864315000	-1.135098000	1.608654000
7	-1.818182000	-0.442620000	1.954572000	7	0.655374000	-1.300144000	2.639575000
13	-0.914930000	-1.950898000	1.407116000	13	-0.396620000	-2.226760000	1.428632000
13	-2.474790000	-0.412922000	0.209098000	13	-0.707166000	-0.052635000	2.534705000
13	-0.696954000	0.872041000	2.374291000	13	2.177583000	-0.716800000	1.921848000
13	1.318862000	2.069082000	1.572613000	13	3.064627000	0.434533000	-0.082322000
7	1.098865000	0.699558000	2.790668000	7	2.952836000	-1.353078000	0.368426000
7	-0.482729000	2.457434000	1.443486000	7	2.606577000	1.053389000	1.597567000
7	2.559144000	0.454156000	-1.962854000	7	0.016202000	1.303586000	-2.628634000
7	2.488932000	2.078135000	0.223105000	7	2.547023000	1.152797000	-1.632493000
13	3.104186000	0.386613000	-0.197608000	13	1.375090000	0.055054000	-2.551441000
13	1.664680000	1.979903000	-1.428340000	13	1.066770000	2.242460000	-1.438225000
13	1.840985000	-2.322888000	0.230689000	13	-0.505176000	-2.094079000	-1.563661000
7	0.795978000	-2.340552000	1.752167000	7	0.186830000	-2.967419000	-0.088066000
13	1.776400000	-0.847750000	2.215867000	13	1.792455000	-2.253144000	-0.649432000
7	3.020774000	-1.046088000	0.862385000	7	1.152461000	-1.694082000	-2.289797000
13	-1.028949000	0.844001000	-2.203844000	13	-1.124214000	2.234447000	0.640830000
7	-2.273331000	1.043357000	-0.855701000	7	-0.487330000	1.703874000	2.292881000
13	-1.088891000	2.311172000	-0.228164000	13	1.166004000	2.108514000	1.577409000
7	-0.049090000	2.347103000	-1.755976000	7	0.485332000	2.962154000	0.086402000
6	-5.315254000	0.461325000	-0.206091000	6	-5.186184000	0.447679000	-0.104526000
1	-4.710085000	1.131701000	-0.811585000	1	-6.277332000	0.355548000	-0.096069000
9	-4.422126000	-0.564810000	0.257814000	1	-4.687842000	1.407797000	-0.293879000
1	-5.709164000	0.938337000	0.686255000	8	-4.514290000	-0.545730000	0.099991000
1	-6.085452000	-0.055796000	-0.769797000				
(CH ₃) ₂ O/Al ₁₂ N ₁₂				CH ₃ NH ₂ /Al ₁₂ N ₁₂			
13	-2.389184000	0.020680000	0.184656000	13	0.344867000	-2.646898000	-0.014722000
13	-1.152594000	1.940726000	-0.872344000	13	-1.794366000	-2.091789000	1.106920000
7	-1.943747000	0.449892000	-1.600319000	7	-1.415809000	-2.712766000	-0.590229000
7	-1.797917000	1.682866000	0.830664000	7	-0.092254000	-2.374554000	1.763389000
7	-1.830255000	-1.547984000	0.905107000	7	1.722273000	-1.930170000	-0.883752000
7	0.633012000	-2.649688000	1.318298000	7	2.115365000	0.709427000	-1.488034000
13	-0.590453000	-2.500337000	-0.061600000	13	1.142734000	-0.712167000	-2.134171000
13	-0.470022000	-1.406795000	2.136408000	13	2.527163000	-0.446423000	-0.050701000
13	2.227751000	-1.982110000	0.889804000	13	1.042662000	2.074996000	-1.100097000
13	3.290217000	-0.009008000	-0.160411000	13	-1.090044000	2.669484000	0.012540000
7	2.841011000	-1.672981000	-0.827312000	7	-0.663318000	2.373310000	-1.759240000
7	2.986263000	-0.456265000	1.606504000	7	0.662918000	2.725368000	0.591068000
7	0.431110000	2.642047000	-1.317146000	7	-2.850201000	-0.701794000	1.488467000
7	2.897999000	1.557441000	-0.920254000	7	-2.460941000	1.926857000	0.884828000
13	1.525788000	1.413703000	-2.152151000	13	-3.112025000	0.416797000	0.040631000
13	1.655329000	2.516760000	0.058264000	13	-1.903830000	0.728744000	2.178338000
13	-0.722387000	-0.593928000	-2.366389000	13	-1.756729000	-1.501114000	-1.853583000
7	-0.191009000	-2.269283000	-1.786269000	7	-0.483734000	-0.642512000	-2.876836000
13	1.514999000	-1.604505000	-2.022892000	13	-1.404700000	0.884292000	-2.403262000
7	0.970468000	-0.091769000	-2.930965000	7	-2.844809000	-0.016081000	-1.670101000
13	-0.463657000	1.596275000	2.006108000	13	0.651245000	-0.874515000	2.386167000

7	0.084967000	0.092139000	2.933555000	7	2.080359000	0.019252000	1.651481000
13	1.773602000	0.598648000	2.386756000	13	1.000374000	1.494222000	1.840500000
7	1.250984000	2.261217000	1.776427000	7	-0.272114000	0.650511000	2.887581000
8	-4.306015000	0.024284000	0.287224000	7	4.508812000	-0.660769000	-0.089537000
6	-4.982290000	-1.202057000	-0.024980000	1	4.794846000	-1.297674000	0.651271000
1	-4.382343000	-1.998173000	0.410994000	1	4.777996000	-1.090543000	-0.972248000
1	-5.977327000	-1.173782000	0.420501000	6	5.171809000	0.656050000	0.079615000
1	-5.049174000	-1.314603000	-1.110053000	1	4.830842000	1.305013000	-0.725935000
6	-4.969447000	1.200071000	-0.200886000	1	4.845965000	1.072514000	1.032247000
1	-5.985234000	1.214940000	0.195750000	1	6.258089000	0.568669000	0.062103000
1	-4.398584000	2.047334000	0.174289000				
1	-4.971056000	1.187078000	-1.292841000				

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