

How can carbon favor the planar multi-coordination in boron-based clusters?

Global structures of $CB_xE_y^{2-}$ (E=Al, Ga, $x+y=4$)

Supporting Information.

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I: Full citations for reference.

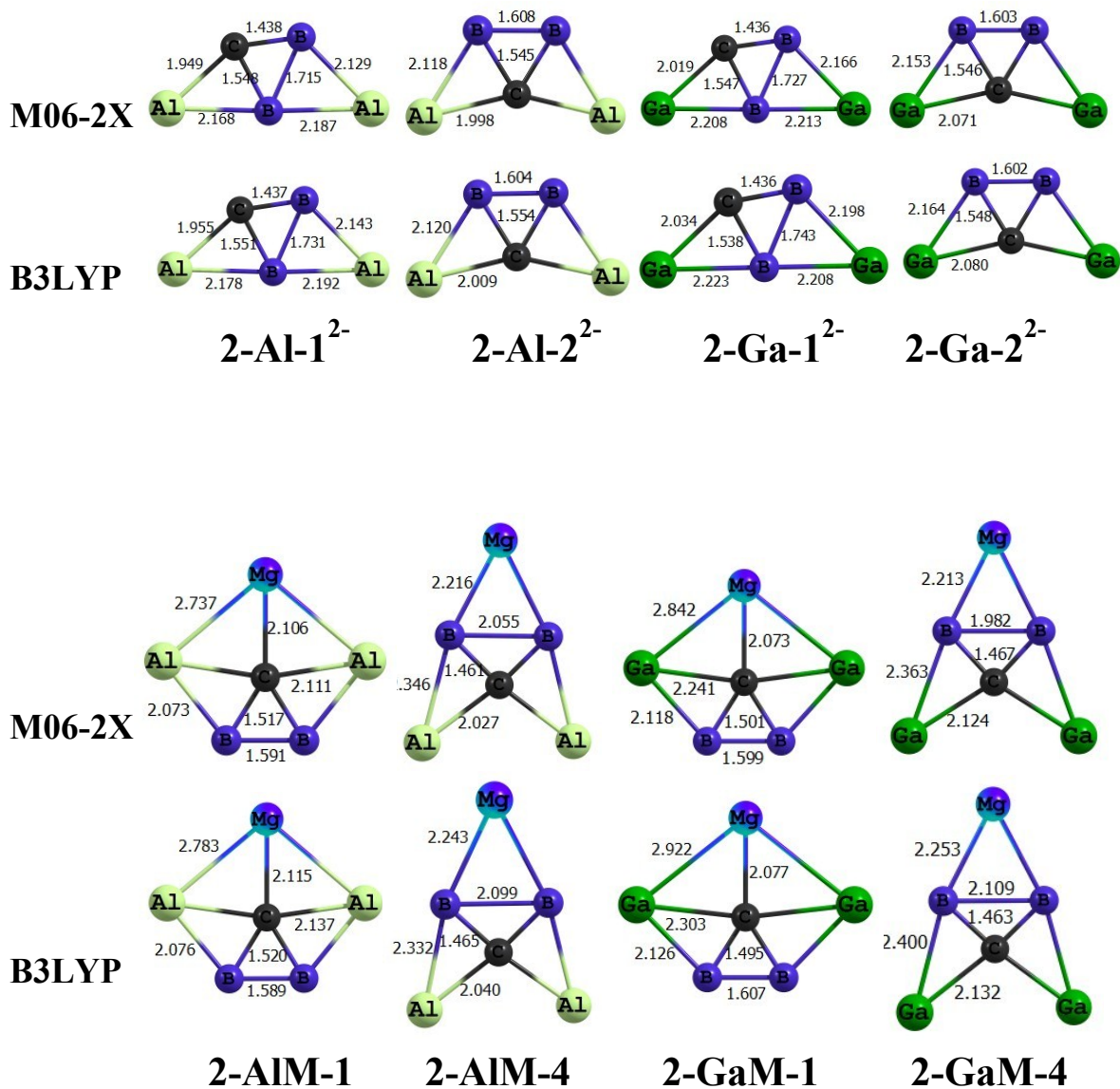
II. Geometrical information at the M06-2X and B3LYP methods.

III. T1 diagnostic values

IV: Coordinates and absolute energies (a.u.) of the low-lying isomers of $CB_xE_y^{2-}$ (E=Al, Ga, $x+y=4$)

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision A.02*. Gaussian, Inc., Wallingford CT, 2009.

II. Figure S1. The geometrical information obtained at the M06-2X and B3LYP with aug-cc-pVTZ basis set.



III. Table S1. T1 diagnostic values computed for the global minimum and the closest isomers.

T1	CB ₄ ²⁻	CB ₃ Al ²⁻	CB ₃ Ga ²⁻	CB ₂ Al ₂ ²⁻	CB ₂ Ga ₂ ²⁻	CBA ₃ ²⁻	CBGa ₃ ²⁻
01	0.071	0.025	0.023	0.020	0.017	0.021	0.018
02	0.074	0.028	0.030	0.022	0.018	0.025	0.022

T1	CB ₃ AlMg	CB ₃ GaMg	CB ₂ Al ₂ Mg	CB ₂ Ga ₂ Mg	CBA ₃ Mg	CBGa ₃ Mg
01	0.026	0.024	0.025	0.020	0.021	0.018
02	0.026	0.022	0.024	0.020	0.027	0.021

IV. Coordinates and absolute energies of CB_xE_y²⁻ and CB_xE_yMg (E=Al, Ga, x+y=4) systems obtained at the (U)B3LYP/aug-cc-pVTZ level.

S1-1. CB_xE_y²⁻

0-1²⁻ HF=-137.2426456
 6 1.479652000 -0.370948000 -0.058468000
 5 0.715248000 0.816430000 0.167296000
 5 0.000104000 -0.695565000 -0.035083000
 5 -0.889506000 0.834463000 -0.162482000
 5 -1.601427000 -0.510190000 0.100430000

0-2²⁻ HF=-137.2379202
 5 1.630305000 -0.433924000 0.051686000
 6 0.695245000 0.642354000 -0.161562000
 5 -0.060860000 -0.733578000 0.072297000
 5 -0.727253000 0.834245000 0.181301000
 5 -1.676487000 -0.437568000 -0.111410000

0-3²⁻ HF=-137.225684
 5 0.000000000 1.544966000 0.612044000
 5 0.000000000 0.792436000 -0.888620000
 6 0.000000000 0.000000000 0.460961000
 5 0.000000000 -0.792436000 -0.888620000
 5 0.000000000 -1.544966000 0.612044000

1-Al-1²⁻ HF=-354.9191379
 5 -1.342602000 1.820894000 0.000000000
 6 -1.497446000 0.352397000 0.000000000
 5 -0.699417000 -0.844878000 0.000000000
 13 1.476521000 -0.829739000 0.000000000
 5 0.000000000 0.758430000 0.000000000

1-Al-2⁻ HF=-354.9072236
5 0.946499000 -0.650127000 0.000000000
6 0.000000000 0.586993000 0.000000000
5 1.549273000 0.829030000 0.000000000
5 0.410885000 2.055710000 0.000000000
13 -1.117945000 -1.130386000 0.000000000

1-Al-3⁻ HF=-354.9078776
5 -1.232651000 1.972902000 0.000000000
5 -1.619669000 0.354549000 0.000000000
13 1.366233000 -0.901902000 0.000000000
6 -0.583239000 -0.648202000 0.000000000
5 0.000000000 0.795338000 0.000000000

1-Ga-1⁻ HF=-2037.4115353
5 -0.937885000 -2.662515000 0.000000000
6 0.419371000 -2.077743000 0.000000000
5 -0.659049000 -0.973134000 0.000000000
5 1.093689000 -0.807863000 0.000000000
31 0.000000000 1.118839000 0.000000000

1-Ga-2⁻ HF=-2037.3978392
5 1.136479000 -2.359509000 0.000000000
5 -0.534399000 -2.275721000 0.000000000
6 0.419543000 -1.035537000 0.000000000
5 -1.105532000 -0.777276000 0.000000000
31 0.000000000 1.073411000 0.000000000

1-Ga-3⁻ HF=-2037.3911656
5 -0.635926000 1.154308000 -0.160545000
5 -2.127709000 0.696226000 0.182440000
31 1.104332000 -0.073437000 0.012019000
6 -2.535018000 -0.705978000 -0.057686000
5 -1.041204000 -0.548051000 -0.027189000

2-Al-1⁻ HF=-572.5882887
13 -2.173414000 0.271853000 0.000000000
5 0.000000000 0.419810000 0.000000000
6 -0.671034000 -0.978729000 0.000000000
5 0.757074000 -1.136402000 0.000000000
13 2.191940000 0.455481000 0.000000000

2-Al-2⁻ HF=-572.5799862
13 0.000000000 1.958800000 0.486452000
6 0.000000000 0.000000000 0.041590000
5 0.000000000 0.801821000 -1.289729000
5 0.000000000 -0.801821000 -1.289729000
13 0.000000000 -1.958800000 0.486452000

2-Al-3⁻ HF=-572.5760203
5 -2.520162000 -0.614594000 0.000109000

6	-1.128679000	-0.956814000	0.000333000
5	0.283954000	-0.984711000	0.000064000
13	2.155778000	-0.057291000	-0.000172000
13	-0.774769000	1.114015000	-0.000047000

2-Ga-1²⁻ HF=-3937.5686112

31	2.216172000	0.035952000	0.000000000
5	0.000000000	0.203680000	0.000000000
6	0.607664000	-1.208995000	0.000000000
5	-0.823423000	-1.332216000	0.000000000
31	-2.200974000	0.380069000	0.000000000

2-Ga-2²⁻ HF=-3937.5566752

31	0.000000000	2.029280000	-0.263543000
5	0.000000000	0.800783000	1.518215000
6	0.000000000	0.000000000	0.192922000
5	0.000000000	-0.800783000	1.518215000
31	0.000000000	-2.029280000	-0.263543000

2-Ga-3²⁻ HF=-3937.5673814

5	-2.822683000	1.036211000	0.000000000
31	-1.116704000	-0.875822000	0.000000000
6	-1.411384000	1.286727000	0.000000000
5	0.000000000	1.280066000	0.000000000
31	1.845146000	0.253185000	0.000000000

2-Ga-4²⁻ HF=-3937.5619216

6	-0.001967000	2.600636000	-0.000242000
5	-0.781607000	1.498954000	0.455199000
5	0.778656000	1.499270000	-0.454862000
31	-1.410874000	-0.494206000	-0.040573000
31	1.411731000	-0.492727000	0.040565000

2-Ga-5²⁻ HF=-3937.5541261

5	-1.048968000	2.525610000	0.000000000
5	0.000000000	1.134991000	0.000000000
31	1.769731000	0.025718000	0.000000000
31	-1.308701000	-0.841211000	0.000000000
6	-1.507853000	1.162883000	0.000000000

3-Al-1²⁻ HF=-790.2375371

13	1.974545000	0.600727000	0.000000000
5	0.000006000	1.543700000	0.000000000
13	-1.974541000	0.600743000	0.000000000
13	-0.000007000	-1.833662000	0.000000000
6	0.000000000	0.083333000	0.000000000

3-Al-2²⁻ HF=-790.2414395

13	-1.745934000	1.852761000	0.000000000
6	0.000000000	1.080047000	0.000000000
5	1.166146000	0.301147000	0.000000000

13	2.081445000	-1.598928000	0.000000000
13	-0.784029000	-0.868141000	0.000000000

3-Al-3²⁻ HF=-790.2337962

6	0.915331000	-0.730362000	0.000000000
5	0.000000000	0.398188000	0.000000000
13	-1.901565000	1.246647000	0.000000000
13	-0.805206000	-1.693524000	0.000000000
13	2.284310000	0.630818000	0.000000000

3-Ga-1²⁻ HF=-5837.7117681

5	0.000005000	1.602902000	0.000000000
31	2.049788000	0.758439000	0.000000000
6	0.000000000	0.150276000	0.000000000
31	-0.000006000	-1.804513000	0.000000000
31	-2.049784000	0.758455000	0.000000000

3-Ga-2²⁻ HF=-5837.7224937

6	-0.722490000	-0.947695000	0.000000000
5	0.664453000	-1.151350000	0.000000000
31	2.621807000	-0.329282000	0.000000000
31	0.000000000	1.111048000	0.000000000
31	-2.589140000	-0.412639000	0.000000000

S1-2. CB_xE_yMg

0-Mg-1 HF=-337.4058032

6	-0.386397000	0.083438000	0.562375000
5	0.625527000	1.025162000	0.086660000
5	0.870081000	-0.658409000	0.136098000
5	2.094854000	0.640131000	-0.322670000
5	2.392002000	-0.834756000	-0.118936000
12	-2.299495000	-0.113439000	-0.190001000

0-Mg-2 HF=-337.402244

6	-2.320167000	-0.652631000	-0.161530000
5	-0.915617000	-0.650421000	0.206183000
5	-1.871869000	0.649394000	-0.474338000
5	0.450029000	-0.010405000	0.823253000
5	-0.499804000	1.074381000	0.236854000
12	2.342276000	-0.116580000	-0.249215000

0-Mg-3 HF=-337.397251

5	0.060100000	-0.102561000	-1.406480000
5	0.060100000	-1.640298000	-0.798561000
6	0.567387000	-0.408904000	0.000000000
5	0.060100000	-1.640298000	0.798561000
5	0.060100000	-0.102561000	1.406480000
12	-0.383859000	1.656834000	0.000000000

1-AlM-1 HF=-555.0626901

5	-1.440879000	1.059341000	-0.015055000
6	-0.043522000	0.492878000	0.181053000
5	-0.176348000	2.031706000	-0.075236000
5	1.257869000	1.284031000	-0.028811000
13	-1.338571000	-1.084790000	-0.022077000
12	1.621612000	-0.894200000	-0.016984000

1-AIM-2 HF=-555.0600657

5	-1.847856000	0.838640000	0.000000000
5	0.000000000	0.505716000	0.000000000
13	1.665909000	-2.256746000	0.000000000
6	0.155140000	-0.965345000	0.000000000
5	-1.263173000	-0.640749000	0.000000000
12	-0.586042000	2.634311000	0.000000000

1-AIM-3 HF=-555.0580934

5	-0.958266000	0.191058000	0.001004000
6	0.169341000	1.111745000	0.000169000
5	0.568163000	-0.398725000	0.000860000
5	1.595961000	1.204836000	-0.000588000
13	-3.074294000	-0.307840000	-0.000359000
12	2.743374000	-0.637867000	-0.000227000

1-AIM-4 HF=-555.0652293

5	0.507670000	-0.908910000	0.000000000
6	-0.904164000	-0.701033000	0.000000000
5	-1.748524000	0.477098000	0.000000000
13	-1.128016000	2.528915000	0.000000000
5	0.000000000	0.610016000	0.000000000
12	2.191122000	-2.463393000	0.000000000

1-AIM-5 HF=-555.0530811

5	0.791667000	1.409359000	0.007904000
13	2.040964000	-0.365756000	-0.143040000
5	-0.095720000	-1.243803000	0.229527000
5	-0.830763000	1.414674000	-0.051761000
6	0.054341000	0.189394000	0.424096000
12	-2.182042000	-0.356890000	-0.134450000

1-AIM-6 HF=-555.0571829

5	0.402421000	-1.031302000	0.000000000
5	-1.140834000	-0.720902000	0.000000000
13	-0.948095000	2.530648000	0.000000000
6	-1.564327000	0.657008000	0.000000000
5	0.000000000	0.517698000	0.000000000
12	2.116939000	-2.555661000	0.000000000

1-AIM-7 HF=-555.0570219

5	0.932479000	1.764959000	0.000000000
6	0.000000000	0.444088000	0.000000000
5	1.608915000	0.328495000	0.000000000

5	0.600082000	-0.881370000	0.000000000
13	-1.150697000	2.167091000	0.000000000
12	-0.062359000	-3.074761000	0.000000000

1-GaM-1 HF=-2237.5536658

5	-2.308764000	0.474767000	-0.070977000
5	-1.483118000	1.864848000	-0.095965000
6	-0.786354000	0.486036000	0.206601000
5	0.094893000	1.693100000	0.033754000
31	1.308938000	-0.147628000	-0.016415000
12	-1.447836000	-1.541943000	-0.005401000

1-GaM-2 HF=-2237.5565576

5	2.677932000	0.657134000	0.000000000
5	1.190294000	-0.483849000	0.000000000
5	1.191003000	1.223927000	0.000000000
6	0.000000000	0.386646000	0.000000000
31	-2.039815000	0.274402000	0.000000000
12	3.161510000	-1.484366000	0.000000000

1-GaM-3 HF=-2237.5601976

5	2.742848000	0.327432000	0.000000000
6	1.363856000	0.707327000	0.000000000
5	1.250908000	-0.851832000	0.000000000
5	0.000000000	0.194168000	0.000000000
31	-2.158509000	0.608513000	0.000000000
12	3.230154000	-1.788058000	0.000000000

1-GaM-4 HF=-2237.559468

5	1.230676000	1.390195000	0.000000000
6	1.553218000	0.006403000	0.000000000
5	0.000000000	0.375762000	0.000000000
5	0.759364000	-1.215283000	0.000000000
31	-1.430582000	-1.448165000	0.000000000
12	2.089877000	3.508444000	0.000000000

1-GaM-5 HF=-2237.5445679

5	-0.658857000	0.228585000	0.924298000
5	-2.278948000	-0.071769000	0.754030000
31	1.019585000	-0.671118000	-0.010027000
6	-2.712557000	-0.433244000	-0.516863000
5	-1.322637000	-0.312268000	-0.661389000
12	0.497535000	2.015115000	-0.139390000

1-GaM-6 HF=-2237.55173

5	0.000000000	0.302477000	0.000000000
5	1.313006000	-0.675960000	0.000000000
31	-2.190980000	0.566976000	0.000000000
6	2.664080000	0.194411000	0.000000000
5	1.456787000	0.976706000	0.000000000
12	3.173911000	-1.813236000	0.000000000

1-GaM-7 HF=-2237.5488972
5 -3.291651000 -0.130275000 0.000003000
6 -2.873475000 -1.478194000 0.000029000
5 -1.550108000 -1.022874000 -0.000071000
31 2.052337000 -0.064327000 0.000000000
5 -0.151352000 -0.218853000 0.000044000
12 -1.784671000 1.476942000 -0.000003000

2-AIM-1 HF=-772.7185921
13 0.000000000 2.114495000 -0.071325000
6 0.000000000 0.000000000 -0.377720000
5 0.000000000 0.794403000 -1.673209000
5 0.000000000 -0.794403000 -1.673209000
13 0.000000000 -2.114495000 -0.071325000
12 0.000000000 0.000000000 1.737740000

2-AIM-2 HF=-772.7185902
13 1.349916000 1.432292000 -0.020941000
6 -0.226095000 0.011545000 0.105474000
5 -0.775016000 1.351970000 0.036544000
13 -2.397201000 -0.170897000 -0.038095000
5 -0.474117000 -1.414805000 0.040137000
12 1.768079000 -1.346102000 -0.020731000

2-AIM-3 HF=-772.7212229
13 0.211553000 -2.358274000 0.000000000
5 0.000000000 0.397515000 0.000000000
6 -0.912188000 -0.758408000 0.000000000
5 -1.743108000 0.405644000 0.000000000
13 -1.137341000 2.520818000 0.000000000
12 2.185326000 -0.131535000 0.000000000

2-AIM-4 HF=-772.7134093
5 0.000000000 1.049531000 0.761875000
13 0.000000000 1.619878000 -1.499744000
6 0.000000000 0.000000000 -0.260072000
13 0.000000000 -1.619878000 -1.499744000
5 0.000000000 -1.049531000 0.761875000
12 0.000000000 0.000000000 2.744586000

2-AIM-5 HF=-772.7189442
13 2.755683000 -1.046440000 0.000000000
5 0.351646000 -0.793961000 0.000000000
6 1.337740000 0.360178000 0.000000000
5 0.000000000 0.835742000 0.000000000
13 -1.702655000 -0.908014000 0.000000000
12 -1.956170000 1.919826000 0.000000000

2-AIM-6 HF=-772.7199097
13 3.015529000 -0.126074000 0.000000000

5	0.000000000	0.365698000	0.000000000
6	1.088404000	-0.576363000	0.000000000
5	0.064834000	-1.601804000	0.000000000
13	-1.583356000	1.817615000	0.000000000
12	-2.122737000	-1.029277000	0.000000000

2-AIM-7 HF=-772.7175032

13	2.868121000	-0.356675000	0.000000000
5	0.000000000	0.143970000	0.000000000
6	0.982602000	-0.928197000	0.000000000
5	-0.341306000	-1.536145000	0.000000000
13	-2.210018000	-0.605214000	0.000000000
12	-1.062035000	2.086218000	0.000000000

2-AIM-8 HF=-772.7166084

5	-1.767196000	-1.342523000	0.000000000
6	-0.359175000	-1.186181000	0.000000000
5	1.040036000	-1.061653000	0.000000000
13	2.989459000	-0.074847000	0.000000000
13	0.000000000	0.947314000	0.000000000
12	-2.756010000	0.649658000	0.000000000

2-AIM-9 HF=-772.7123619

13	-0.294838000	-1.574929000	0.000000000
6	0.000000000	0.347827000	0.000000000
5	1.114349000	1.413207000	0.000000000
5	-0.439893000	1.783557000	0.000000000
13	-2.123842000	0.539554000	0.000000000
12	2.339213000	-0.384241000	0.000000000

2-AIM-10 HF=-772.712614

13	-1.910407000	1.394203000	0.000000000
5	-0.814353000	-0.515560000	0.000000000
6	0.000000000	0.770865000	0.000000000
5	0.828148000	-0.493043000	0.000000000
13	-0.023828000	-2.541804000	0.000000000
12	2.089674000	1.278053000	0.000000000

2-AIM-11 HF=-772.7098974

13	-1.710812000	-0.900953000	0.000000000
5	0.368499000	-0.714989000	0.000000000
6	0.000000000	0.720426000	0.000000000
5	1.433991000	0.666778000	0.000000000
13	2.678522000	-1.155492000	0.000000000
12	-1.799390000	1.887690000	0.000000000

2-AIM-12 HF=-772.7126541

5	1.369470000	0.008109000	0.000409000
6	0.296923000	-0.893936000	-0.000173000
5	-1.098990000	-1.035863000	-0.000376000
13	-3.176238000	-0.255953000	0.000239000

13	-0.440581000	1.225845000	-0.000201000
12	3.657059000	-0.175516000	0.000031000

2-GaM-1 HF=-4137.7058197

31	2.288294000	0.055287000	0.000000000
5	0.803798000	1.576724000	0.000000000
6	0.000000000	0.316100000	0.000000000
5	-0.803167000	1.577186000	0.000000000
31	-2.288282000	0.056290000	0.000000000
12	-0.000294000	-1.760418000	0.000000000

2-GaM-2 HF=-4137.7101058

31	1.820015000	-0.776480000	-0.067044000
5	-0.565996000	1.549415000	0.296470000
5	-0.263851000	-1.161744000	0.360738000
31	-2.287545000	-0.114229000	-0.111133000
6	-0.085174000	0.239658000	0.629924000
12	1.596142000	2.019640000	-0.128508000

2-GaM-3 HF=-4137.716336

31	-1.484465000	-1.976982000	0.000000000
5	0.000000000	0.426964000	0.000000000
6	0.289578000	-1.007170000	0.000000000
5	1.570429000	-0.383577000	0.000000000
31	2.030469000	1.808789000	0.000000000
12	-2.209644000	0.920006000	0.000000000

2-GaM-4 HF=-4137.7039268

31	0.000000000	1.688844000	-0.918029000
5	0.000000000	1.054594000	1.396713000
6	0.000000000	0.000000000	0.382733000
5	0.000000000	-1.054594000	1.396713000
31	0.000000000	-1.688844000	-0.918029000
12	0.000000000	0.000000000	3.387853000

2-GaM-5 HF=-4137.7107406

31	2.414434000	1.238878000	0.000000000
5	0.000000000	0.420307000	0.000000000
6	1.228804000	-0.458572000	0.000000000
5	0.056557000	-1.252812000	0.000000000
31	-2.039731000	0.051839000	0.000000000
12	-1.605952000	-2.758187000	0.000000000

2-GaM-6 HF=-4137.7175591

5	1.925116000	-0.256966000	0.000000000
5	0.000000000	0.298604000	0.000000000
31	-1.031527000	2.235584000	0.000000000
31	-0.138704000	-2.836600000	0.000000000
6	0.666774000	-0.970738000	0.000000000
12	1.887579000	2.020645000	0.000000000

2-GaM-7 HF=-4137.7105063
31 2.569343000 -1.365694000 0.000000000
5 0.000000000 0.625689000 0.000000000
6 0.672521000 -0.640338000 0.000000000
5 -0.766604000 -0.934407000 0.000000000
31 -2.362767000 0.452551000 0.000000000
12 -0.550497000 2.807752000 0.000000000

2-GaM-8 HF=-4137.7162412
5 2.203253000 1.822600000 0.000307000
6 0.827863000 1.491321000 0.000363000
5 -0.538646000 1.188481000 0.000366000
31 -2.438470000 0.054768000 -0.000235000
31 0.703321000 -0.804089000 0.000336000
12 3.374950000 -0.064532000 -0.000723000

2-GaM-9 HF=-4137.7061336
5 2.764488000 -0.000002000 -0.234952000
6 2.235415000 -0.000002000 -1.530143000
5 0.943971000 -0.000001000 -1.008257000
31 -0.791926000 -1.247771000 -0.047441000
31 -0.791924000 1.247772000 -0.047442000
12 1.428714000 0.000000000 1.528188000

2-GaM-10 HF=-4137.7040977
5 2.326927000 -0.575990000 0.622837000
31 1.079887000 0.527291000 -0.693899000
6 1.679193000 -1.373718000 1.556389000
5 0.461377000 -0.969901000 1.015312000
31 -1.403557000 -0.635015000 -0.351869000
12 -1.165244000 1.609265000 1.240811000

2-GaM-11 HF=-4137.708308
31 1.927287000 -0.608299000 0.000000000
5 0.000000000 0.286598000 0.000000000
6 -0.509969000 -1.086391000 0.000000000
5 -1.681099000 -0.258607000 0.000000000
31 -1.724375000 1.983089000 0.000000000
12 0.431252000 -3.020008000 0.000000000

2-GaM-12 HF=-4137.7085195
5 -2.718907000 0.518131000 0.000000000
31 -1.877958000 -1.405632000 0.000000000
6 -1.383012000 0.942424000 0.000000000
5 0.000000000 1.163875000 0.000000000
31 2.200358000 1.435555000 0.000000000
12 0.991519000 -1.249347000 0.000000000

2-GaM-13 HF=-4137.7111419
5 2.073912000 0.386907000 0.000000000
31 0.000000000 1.261066000 0.000000000

6	1.271559000	-0.763830000	0.000000000
5	-0.025856000	-1.278691000	0.000000000
31	-2.257211000	-1.265856000	0.000000000
12	4.341993000	0.765865000	0.000000000

3-AIM-1 HF=-990.3731681

13	-1.246553000	2.017423000	0.000000000
5	0.767213000	1.358151000	0.000000000
13	2.305677000	-0.036752000	0.000000000
13	-1.818759000	-0.646385000	0.000000000
6	0.000000000	0.157377000	0.000000000
12	0.503265000	-2.090061000	0.000000000

3-AIM-2 HF=-990.3785093

13	-1.650090000	-0.799088000	0.000000000
5	1.064576000	-0.630425000	0.000000000
13	1.830317000	1.429536000	0.000000000
13	-0.971793000	2.057184000	0.000000000
6	0.000000000	0.307312000	0.000000000
12	0.413956000	-2.802580000	0.000000000

3-AIM-3 HF=-990.3808472

13	0.272912000	-1.942098000	0.000000000
6	1.172626000	-0.211676000	0.000000000
5	0.000000000	0.549794000	0.000000000
13	-1.597648000	2.009390000	0.000000000
13	2.983289000	0.519185000	0.000000000
12	-2.383079000	-0.758593000	0.000000000

3-GaM-1 HF=-6037.8625728

5	1.280932000	-0.451943000	0.000000000
31	-0.007927000	-2.202766000	0.000000000
6	0.000000000	0.145614000	0.000000000
31	-2.029363000	-0.157494000	0.000000000
31	2.065499000	1.514066000	0.000000000
12	-0.606594000	2.301504000	0.000000000

3-GaM-2 HF=-6037.8669503

5	1.411238000	-0.007489000	0.000000000
31	-0.301498000	2.126883000	0.000000000
6	0.000000000	0.083063000	0.000000000
31	-1.848243000	-0.764210000	0.000000000
31	0.903803000	-2.128124000	0.000000000
12	2.630657000	1.939005000	0.000000000

3-GaM-3 HF=-6037.8731054

31	2.619926000	-0.991953000	0.000000000
5	0.000000000	0.558916000	0.000000000
6	0.644593000	-0.680331000	0.000000000
31	-1.007730000	-1.812565000	0.000000000
31	-0.692557000	2.633350000	0.000000000

12	-2.698032000	0.549468000	0.000000000
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3-GaM-4 HF=-6037.8644645

31	2.889897000	-0.564978000	0.000000000
5	0.000000000	0.615015000	0.000000000
31	-2.194500000	1.051117000	0.000000000
31	-0.758325000	-1.683932000	0.000000000
6	0.898429000	-0.446375000	0.000000000
12	-0.286650000	3.061230000	0.000000000

3-GaM-5 HF=-6037.8630416

6	-1.071295000	0.491869000	0.000176000
31	-2.656126000	-0.758713000	0.000113000
31	1.476769000	1.419369000	0.000449000
31	1.754404000	-1.720044000	-0.000454000
5	0.048042000	-0.344148000	0.002025000
12	-0.969909000	2.634213000	-0.001212000