

Gas phase enthalpies of formation for aminonitroacetylene, aminonitromethane, and diaminodinitromethane: A Gaussian-4 (G4) theoretical study

Sierra Rayne ^{a *}, Kaya Forest ^b

Gas phase (298.15 K, 1 atm) enthalpies of formation were calculated at the Gaussian-4 (G4) level of theory using the atomization energy approach for the proposed high energy materials aminonitroacetylene (284.0 to 285.7 kJ/mol), aminonitromethane (-66.4 to -65.0 kJ/mol), and diaminodinitromethane (-84.0 to -81.6 kJ/mol). The results are in good agreement with prior G2 and G3 level estimates, and should help constrain the actual enthalpies of formation for these potential HEMs.

Keywords: aminonitroacetylene, aminonitromethane, diaminodinitromethane, high energy materials, enthalpy of formation, Gaussian-4 (G4), theoretical study

Aminonitroacetylene (**1**), aminonitromethane (**2**), and diaminodinitromethane (**3**) have been proposed as high energy materials (HEMs; Figure 1) [1–4]. Their gas phase enthalpies of formation ($\Delta_f H_{(g)}^\circ$) have not been experimentally determined, but previous theoretical estimates have been put forward in the literature at the SCF/6-31G, G2, and G3 levels of theory (Table 1). In the current work, we employ the Gaussian-4 (G4) [5] composite method level of theory within Gaussian 09 (G09) [6] and apply the atomization energy approaches in ref. [7] and ref. [8,9] to provide additional $\Delta_f H_{(g)}^\circ$ estimates for these compounds. Three-dimensional visualizations of the G4 optimized geometries are shown in Figure 2, and full G09 archive entries (including geometry coordinates) are provided in the Supporting Information. Excellent agreement was obtained between our G4 $\Delta_f H_{(g)}^\circ$ estimates for **1** and those previously reported at the G2 and G3 levels [4]. The $\Delta_f H_{(g)}^\circ$ estimate of 179.9

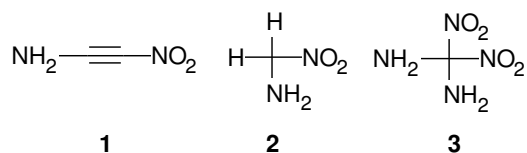


Figure 1: Structures of aminonitroacetylene (**1**), aminonitromethane (**2**), and diaminodinitromethane (**3**).

Table 1: Estimated gas phase enthalpies of formation ($\Delta_f H_{(g)}^\circ$) for aminonitroacetylene (**1**), aminonitromethane (**2**), and diaminodinitromethane (**3**) at various levels of theory. Values are in kJ/mol.

level of theory	1	2	3	ref.
SCF/6-31G	n/a	-72.3	-111.3	[1, 2]
G2	284.0	-73.7	-97.7	[3, 4]
G3	285.6	-60.2	-72.7	[3, 4]
G4 ^a	285.7	-65.0	-81.6	current work
G4 ^b	284.0	-66.4	-84.0	current work

^a atomization energy approach as described in ref. [7]. ^b atomization energy approach as described in ref. [8,9].

kJ/mol for **1** by Golovin and Takhistov [10] appears to be in error when compared to the current G4 calculations and prior G2 and G3 estimates. G4 $\Delta_f H_{(g)}^\circ$ estimates for **2** and **3** reside between the prior G2, G3, and SCF/6-31G estimates [1–4]. The findings presented herein will assist in better constraining the actual $\Delta_f H_{(g)}^\circ$ for these potential HEMs.

Acknowledgements

This work was made possible by the facilities of the Western Canada Research Grid (West-Grid:www.westgrid.ca; project 100185), the Shared Hierarchical Academic Research Computing Network (SHARCNET:www.sharcnet.ca; project sn4612), and Compute/Calcul Canada.

*Corresponding author: Tel/Fax: 1.250.487.0166 Email: rayne.sierra@gmail.com. ^a Ecologica Research, 301-1965 Pandosy Street, Kelowna, British Columbia, Canada, V1Y 1R9. ^b Department of Chemistry, Okanagan College, 583 Duncan Ave West, Penticton, British Columbia, Canada, V2A 8E1.

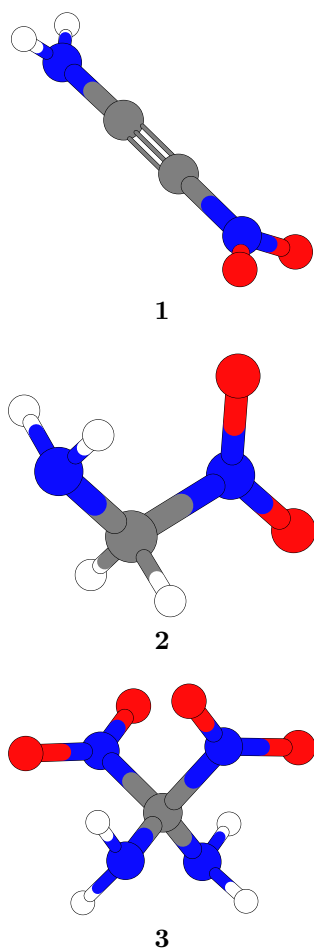


Figure 2: Visualizations of Gaussian-4 (G4) optimized geometries for aminonitroacetylene (1), aminonitromethane (2), and diaminodinitromethane (3).

References

- [1] Sana, G., Leroy, G., Peeters, D., Wilante, C., "The theoretical study of the heats of formation of organic compounds containing the substituents CH₃, CF₃, NH₂, NF₂, NO₂, OH and F," *Journal of Molecular Structure (Theochem)*, 164, 1988, 249-274.
- [2] Leroy, G., Sana, G., Wilante, C., Peeters, D., Bourasseau, S., "Heats of formation of some energetic compounds containing NO₂ and/or NF₂ groups," *Journal of Molecular Structure (Theochem)*, 189, 1989, 251-259.
- [3] Mathews, K.Y., Ball, D.W., "New potential high energy materials: High-level calculations on the properties of aminonitromethanes," *Journal of Molecular Structure (Theochem)*, 868, 2008, 78-81.
- [4] Mathews, K.Y., Ball, D.W., "Calculated thermochemistry of aminonitroacetylene: A new high-energy material?," *Journal of Molecular Structure (Theochem)*, 868, 2008, 78-81.
- [5] Curtiss, L.A., Redfern, P.C., Raghavachari, K., "Gaussian-4 theory," *Journal of Chemical Physics*, 126, 2007, 084108.
- [6] Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G.A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H.P., Izmaylov, A.F., Bloino, J., Zheng, G., Sonnenberg, J.L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, Jr., J.A., Peralta, J.E., Ogliaro, F., Bearpark, M., Heyd, J.J., Brothers, E., Kudin, K.N., Staroverov, V.N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J.C., Iyengar, S.S., Tomasi, J., Cossi, M., Rega, N., Millam, N.J., Klene, M., Knox, J.E., Cross, J.B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R.E., Yazyev, O., Austin, A.J., Cammi, R., Pomelli, C., Ochterski, J.W., Martin, R.L., Morokuma, K., Zakrzewski, V.G., Voth, G.A., Salvador, P., Dannenberg, J.J., Dapprich, S., Daniels, A.D., Farkas, O., Foresman, J.B., Ortiz, J.V., Cioslowski, J., Fox, D.J., *Gaussian 09, Revision A.02*, Gaussian, Inc., Wallingford, CT, USA, 2009.
- [7] Saeys, M., Reyniers, M.F., Marin, G.B., Van Speybroeck, V., Waroquier, M., "Ab initio calculations for hydrocarbons: Enthalpy of formation, transition state geometry, and activation energy for radical reactions," *J. Phys. Chem. A* 2003, 107, 9147-9159.
- [8] Nicolaides, A., Rauk, A., Glukhovtsev, M.N., Radom, L., "Heats of formation from G2, G2(MP2), and G2(MP2,SVP) total energies," *Journal of Physical Chemistry*, 100, 1996, 17460-17464.
- [9] Notario, R., Castano, O., Abboud, J.L.M., Gomperts, R., Frutos, L.M., Palmeiro, R., "Organic thermochemistry at high ab initio levels. 1. A G2(MP2) and G2 study of cyclic saturated and unsaturated hydrocarbons (including

aromatics),” *Journal of Organic Chemistry*, 64, 1999, 9011-9014.

- [10] Golovin, A.V., Takhistov, V.V., “Thermochemistry of organic and heteroorganic species. Part XII. Mono- and disubstituted acetylenes and ethynyl free radicals. New electronegativity scale,” *Journal of Molecular Structure*, 2004, 701, 57-91.

Supporting Information

Gas phase enthalpies of formation for aminonitroacetylene, aminonitromethane, and diaminodinitromethane: A Gaussian-4 (G4) theoretical study

Sierra Rayne^{*,†} and Kaya Forest[†]

Ecologica Research, Kelowna, British Columbia, Canada V1Y 1R9; Department of Chemistry, Okanagan College, Penticton, British Columbia, Canada V2A 8E1

* Corresponding author. E-mail: rayne.sierra@gmail.com.

† Ecologica Research.

† Okanagan College.

Gaussian 09 archive entries

aminonitroacetylene

```

Temperature=                298.150000 Pressure=                1.000000
E(ZPE)=                      0.047377 E(Thermal)=                0.053688
E(CCSD(T))=                  -336.284516 E(Empiric)=                -0.111152
DE(Plus)=                    -0.028017 DE(2DF)=                -0.234974
E(Delta-G3XP)=              -0.405489 DE(HF)=                -0.034161
G4(0 K)=                     -337.050933 G4 Energy=                -337.044622
G4 Enthalpy=                 -337.043678 G4 Free Energy=                -337.080997
\\0,1\C,0,-1.4227070838,0.0420197349,0.0026629758\C,0,-0.21
48814251,0.0172831883,-0.0074111472\N,0,-2.7410264433,0.0568737516,-0.
0222857993\N,0,1.1628798389,-0.0069916316,-0.0074217272\H,0,-3.2575635
994,-0.6905127498,0.4148330501\H,0,-3.2288347916,0.9314874423,-0.13873
62365\O,0,1.7417965374,1.0191123595,-0.3606878927\O,0,1.7052869669,-1.
0526920953,0.3464767769\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1
=-336.2397491\MP4/GTBas1=-336.2963669\CCSD(T)/G3Bas1=-336.2845161\MP2/
GTBas2=-336.2661187\MP4/GTBas2=-336.3243842\MP2/GTBas3=-336.4612863\MP
4/GTBas3=-336.531341\HF/GTLargeXP=-335.4203134\MP2/GTLargeXP=-336.8931
453\HF/GFHFB1=-335.4477981\HF/GFHFB2=-335.4531662\G4=-337.0509328\Freq
Coord=-2.6885267556,0.0794057912,0.005032295,-0.4060670444,0.032660492
6,-0.0140050385,-5.1797893009,0.1074758147,-0.0421140574,2.197524421,-
0.013212269,-0.0140250319,-6.1559030634,-1.3048799883,0.7839208556,-6.
1016134845,1.7602561623,-0.2621734916,3.291518435,1.9258432581,-0.6816
013366,3.2225253454,-1.9892997624,0.6547462198\PG=C01 [X(C2H2N2O2)]\NI
mag=0\\1.53792134,-0.03030562,0.09648692,-0.01425050,-0.00627327,0.078
97084,-0.97870851,0.02014989,0.00977365,1.39573015,0.01943547,-0.02682
763,-0.00137060,-0.02505299,0.10288732,0.00769846,-0.00133399,-0.02952
520,-0.00696436,-0.02217664,0.04467888,-0.45990197,0.00421198,-0.00688
664,-0.06486458,0.00111039,-0.00017703,0.80167971,0.01334405,-0.083677
91,0.01827388,-0.00148955,0.00232090,0.00259452,-0.03144230,0.70247588
,0.01985293,0.01780075,-0.03649105,-0.00778002,0.00272830,0.00900144,-
0.09089184,-0.22362289,0.11828446,-0.04628388,0.00027952,-0.00131340,-
0.24573949,0.00346951,-0.00040923,0.02773827,0.00123980,0.00468655,0.7
1541003,0.00129276,-0.00600764,-0.00273383,0.00340573,-0.04340831,-0.0
0678397,-0.00056496,0.00727425,-0.00062686,0.00171574,0.80900979,0.001
66208,-0.00278620,-0.01312986,-0.00059238,-0.00678059,-0.06092734,-0.0
0061222,-0.00053354,0.00588295,-0.00351790,-0.19605025,0.30140263,-0.0
3447143,-0.02487381,0.01564543,0.00512145,-0.00117776,-0.00003514,-0.1
5167052,-0.13985491,0.08962987,-0.00108578,0.00086258,-0.00055736,0.16
996940,-0.00875841,0.00785605,-0.00488244,0.00885900,-0.00028991,0.000
66004,-0.13243312,-0.27205640,0.14226957,-0.00378837,0.00047415,0.0002
1439,0.15123685,0.28052865,-0.00487724,-0.00700612,-0.00160406,-0.0002
7875,0.00078557,0.00107039,0.10016001,0.15850781,-0.08562670,-0.000386
39,0.00033900,0.00087290,-0.09582287,-0.15066220,0.08846451,-0.0332384
7,0.03064279,-0.00327934,0.00487034,0.00073674,-0.00069182,-0.14120183
,0.15842973,-0.01410265,-0.00100160,-0.00098075,0.00007067,0.01243411,
-0.01697054,0.00131504,0.15851033,0.00536889,0.00897347,-0.00399040,-0
.00735692,-0.00027685,0.00048244,0.15881609,-0.35819041,0.06256209,0.0
0280321,0.00029943,0.00021274,0.01335286,-0.01596327,-0.00198971,-0.17
144365,0.36562586,-0.00959413,-0.00139167,-0.00395420,0.00524742,0.000
25658,0.00130866,-0.00175341,0.04591856,-0.00996275,-0.00264102,0.0001
3281,0.00096400,-0.00877947,0.01237207,-0.00275023,0.01647163,-0.05730
482,0.01482718,0.00750514,-0.00158093,0.00068107,-0.06006990,-0.047648
88,0.01681310,-0.00594252,0.00209716,-0.00147111,-0.23032142,-0.188807
42,0.06525459,0.00022883,0.00087350,0.00000375,-0.00056076,-0.00085642
,0.00052660,0.24217072,0.01063249,0.00152560,0.00072897,-0.05645492,-0

```

.01531763,0.01305781,-0.00506840,0.00056083,-0.00151649,-0.14510102,-0.37813692,0.10171640,0.00041895,0.00068564,0.00052349,-0.00008070,-0.00089843,0.00013240,0.21810948,0.47644188,-0.00393858,0.00054681,0.0027589,0.01982509,0.01292722,0.01717287,0.00185716,-0.00071217,-0.00012494,0.05036066,0.10198762,-0.11749719,-0.00001591,0.00027689,0.00095160,-0.00002041,-0.00010830,-0.00168045,-0.07563226,-0.15342698,0.08323497,0.00717779,0.00147619,-0.00037027,-0.05633947,0.04912753,-0.01623397,-0.00583656,-0.00232400,0.00007627,-0.21871613,0.18307631,-0.06170746,-0.00052606,0.00098109,-0.00011355,0.00018788,-0.00068406,0.00052238,0.04698992,-0.02245586,0.00756426,0.22706263,-0.01100963,0.00167115,0.00024767,0.05793977,-0.01908789,0.01349979,0.00537032,0.00129286,0.00040553,0.13938160,-0.38950475,0.10400704,0.00003524,-0.00123491,-0.00049785,-0.00033361,0.00043020,-0.00011593,0.01781351,-0.08486096,0.03850891,-0.20919720,0.49129429,0.00344697,0.00044368,0.00295764,-0.01923065,0.01363016,0.01722029,-0.00169601,-0.00042617,-0.00096342,-0.04677927,0.10373547,-0.11756810,-0.00006454,-0.00024832,-0.00137841,0.00023689,0.00013596,0.00124780,-0.00617574,0.03878440,0.01516725,0.07026235,-0.15605516,0.08331696\\0.00002815,0.00000578,0.00003996,0.00004702,-0.00001332,-0.00003823,-0.00002984,0.00000178,-0.00001923,-0.00001243,0.00004852,0.00001269,-0.00000040,-0.00001832,0.00000760,-0.00000160,0.00001701,-0.00000465,-0.00002530,0.00001089,-0.00000998,-0.00000560,-0.00005233,0.00001184\\@

aminonitromethane

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.066845	E(Thermal)=	0.072177
E(CCS(D(T))=	-299.567630	E(Empiric)=	-0.104205
DE(Plus)=	-0.026653	DE(2DF)=	-0.226189
E(Delta-G3XP)=	-0.353823	DE(HF)=	-0.031291
G4(0 K)=	-300.242945	G4 Energy=	-300.237614
G4 Enthalpy=	-300.236670	G4 Free Energy=	-300.271755

\\0,1\C,0,-2.2494801867,-0.1135258982,0.0008494259\N,0,-0.8397611299,-0.132397359,-0.0017266742\N,0,-2.9002591488,1.304507217,-0.0053613886\H,0,-2.6713150962,-0.5807994219,0.8924375796\H,0,-2.6746870501,-0.5902961392,-0.8840729365\H,0,-0.4555373682,0.3324032333,0.8126753636\H,0,-0.4587120969,0.3222222567,-0.8232831328\O,0,-2.1543501448,2.2684089722,-0.0112447331\O,0,-4.1183877784,1.3307671391,-0.0036435039\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-299.5229187\MP4/GTBas1=-299.5763598\CCSD(T)/G3Bas1=-299.5676299\MP2/GTBas2=-299.5477924\MP4/GTBas2=-299.603013\MP2/GTBas3=-299.7350713\MP4/GTBas3=-299.8025488\HF/GTLargeXP=-298.8087288\MP2/GTLargeXP=-300.1137676\HF/GFHFB1=-298.8335775\HF/GFHFB2=-298.8387575\G4=-300.242945\FreqCoord=-4.2509014943,-0.2145328567,0.0016051822,-1.5869185526,-0.2501947492,-0.0032629414,-5.4806955055,2.4651613785,-0.0101315562,-5.0480539465,-1.0975518454,1.6864626162,-5.0544260159,-1.1154980404,-1.6706557315,-0.8608408692,0.6281510766,1.5357338722,-0.8668402369,0.6089118191,-1.5557796507,-4.071131768,4.2866717148,-0.0212494661,-7.7826250103,2.5147854395,-0.0068852245\PG=C01 [X(C1H4N2O2)]\NImag=0\\0.57173921,0.13845202,0.35594045,-0.00059345,0.00134465,0.64483032,-0.27019951,-0.00869507,0.00032964,0.54746511,-0.05739198,-0.05564268,-0.00026318,0.17338012,0.26731586,0.00065811,-0.00035770,-0.11654380,-0.00081912,0.00239274,0.71318710,-0.05941215,-0.00757732,-0.00003184,-0.03471920,0.02552259,-0.00006292,0.94401915,-0.00505868,-0.07323941,-0.00012785,0.01355575,-0.00890284,0.00005402,0.14535221,0.70717028,-0.00002364,-0.00012862,-0.10137019,-0.00000890,0.00001528,0.00475693,-0.00179534,-0.00258175,0.23328068,-0.08341557,-0.04062719,0.07871101,-0.02011450,-0.01312300,0.03238947,0.00308954,0.00470567,-0.01006570,0.10023493,-0.04436174,-0.09061961,0.09342484

,0.00216023,0.00253094,-0.00277863,-0.00875139,-0.02270096,0.03136873,
0.04303082,0.10558420,0.08316579,0.09724850,-0.23877540,0.00075521,-0.
00152530,0.00372958,0.00223790,-0.00057488,0.00229425,-0.09211828,-0.1
0401599,0.24821495,-0.08405264,-0.04184408,-0.07886969,-0.02022377,-0.
01349058,-0.03215032,0.00311891,0.00480984,0.01001305,0.00510189,0.005
18298,0.00912429,0.10094022,-0.04560260,-0.09267917,-0.09481973,0.0021
5683,0.00257682,0.00278257,-0.00890248,-0.02300565,-0.03105378,0.00512
886,0.00795861,0.01145649,0.04442872,0.10781794,-0.08329114,-0.0986687
7,-0.23612341,-0.00067201,0.00158650,0.00380470,-0.00215171,0.00083061
,0.00258635,-0.00926851,-0.01175903,-0.01848993,0.09221375,0.10535646,
0.24529458,-0.02208681,-0.01950381,-0.03643332,-0.10012027,-0.06885448
,-0.09498066,-0.00197365,-0.00317060,-0.00147691,0.00111612,0.00008566
,0.00056865,-0.00608549,0.00044617,0.00138765,0.11893913,0.00939625,-0
.00593169,0.00125318,-0.09756153,-0.10373916,-0.16835054,0.00272345,0.
00378025,0.00246461,-0.00000098,-0.00043175,-0.00066561,-0.00152583,0.
00166026,0.00002741,0.08142005,0.10197074,-0.00188243,0.00068784,0.002
73997,-0.10630404,-0.12880089,-0.30275253,-0.00046384,-0.00198091,-0.0
0022703,-0.00002985,0.00058752,0.00081867,0.00137207,-0.00045763,0.002
29118,0.11691778,0.14864649,0.32216031,-0.02194190,-0.01906314,0.03676
483,-0.09934660,-0.06719348,0.09507228,-0.00196190,-0.00313995,0.00151
267,-0.00609397,0.00043416,-0.00135937,0.00111758,0.00007681,-0.000570
54,0.00650756,0.00791715,-0.01287690,0.11804619,0.00940758,-0.00595767
,-0.00118358,-0.09559322,-0.10009767,0.16624675,0.00272170,0.00377220,
-0.00252161,-0.00155549,0.00166838,-0.00000985,0.00000363,-0.00043265,
0.00067897,0.00800378,0.00390519,-0.01846298,0.07940969,0.09833584,0.0
0184271,-0.00050204,0.00261567,0.10676337,0.12660156,-0.30727610,0.000
44059,0.00193922,-0.00022546,-0.00132341,0.00045981,0.00229826,0.00002
648,-0.00057445,0.00082379,0.01265274,0.01807194,-0.02529300,-0.117154
40,-0.14622308,0.32679361,0.00021709,-0.00227571,0.00005093,0.00526709
,0.00980167,-0.00006419,-0.26865225,-0.20894183,0.00133395,0.00005693,
0.00151127,-0.00108837,0.00005828,0.00153597,0.00107078,0.00196813,-0.
00104763,0.00170185,0.00195223,-0.00106625,-0.00169261,0.34437018,-0.0
3403030,-0.03943870,0.00036464,0.00235961,0.00142476,-0.00001485,-0.19
820456,-0.44855642,0.00217691,0.00140996,-0.00521222,-0.00127399,0.001
41116,-0.00516995,0.00131840,0.00123293,-0.00066241,-0.00003152,0.0012
2336,-0.00064974,0.00003329,0.27884568,0.47836844,0.00020401,0.0003221
0,0.02411357,-0.00002282,-0.00002794,-0.00095781,0.00127991,0.00219327
,-0.06917899,0.00067088,-0.00332518,-0.00067100,-0.00068857,0.00336007
,-0.00071825,0.00086847,-0.00100767,0.00020262,-0.00088261,0.00102283,
0.00020569,-0.00186336,-0.00267395,0.02317074,-0.03084771,0.00113429,0
.00007187,-0.00800835,0.01134913,-0.00004264,-0.58350844,0.05188758,0.
00051081,0.00002465,0.00070802,-0.00128581,0.00002502,0.00073171,0.001
28173,0.00173528,-0.00132093,0.00156536,0.00172081,-0.00133141,-0.0015
5547,-0.08523766,-0.05424783,0.00043409,0.70409640,0.02918945,0.007568
49,0.00000703,0.00823728,-0.00546603,0.00002564,0.04711579,-0.13831744
,0.00026023,0.00103135,0.00122241,-0.00063936,0.00102417,0.00127380,0.
00062945,0.00034030,-0.00055143,-0.00018792,0.00033539,-0.00054388,0.0
0019376,-0.07836317,0.01989625,0.00013647,-0.00891057,0.11491783,-0.00
007996,0.00005404,0.01851325,-0.00002132,0.00002124,0.00205192,0.00054
724,0.00024827,-0.07191654,0.00103439,-0.00396207,0.00058060,-0.001041
06,0.00395000,0.00053099,0.00049560,-0.00043980,0.00005982,-0.00050597
,0.00045255,0.00005753,0.00055103,0.00010107,0.02383343,-0.00097995,-0
.00042529,0.02628900\0.00001508,-0.00003066,-0.00000976,-0.00000206,-
0.00001271,-0.00001449,0.00000453,0.00004540,0.00000215,0.00000277,0.0
0000336,0.00000024,0.00000206,0.00000286,-0.00000309,0.00000722,0.0000
1771,0.00001647,-0.00001254,-0.00000504,0.00000577,-0.00001936,-0.0000
2600,0.00000115,0.00000231,0.00000507,0.00000156\\\@

diaminodinitromethane

Temperature=	298.150000	Pressure=	1.000000
E (ZPE) =	0.085304	E (Thermal) =	0.094283
E (CCSD (T)) =	-558.787412	E (Empiric) =	-0.180622
DE (Plus) =	-0.049166	DE (2DF) =	-0.399500
E (Delta-G3XP) =	-0.643494	DE (HF) =	-0.056795
G4 (0 K) =	-560.031684	G4 Energy =	-560.022705
G4 Enthalpy =	-560.021760	G4 Free Energy =	-560.066065

\\0,1\C,0,-0.0858300051,0.4866456209,0.2008400951\N,0,-0.52
26233529,0.7718167347,1.4924757247\N,0,1.1234972634,-0.5416482523,0.11
69403851\N,0,0.3149177757,1.6032941037,-0.5291834312\N,0,-1.246761446,
-0.3676564471,-0.4694786636\H,0,0.185433325,1.2740911148,2.0143637859\
H,0,-0.79745027,-0.0712748932,1.9833977298\O,0,1.5975935883,-0.9182096
209,1.1666109997\O,0,1.4783762088,-0.846930285,-1.0084812707\H,0,0.618
1563512,1.3451535403,-1.461250304\H,0,-0.4238770207,2.2948623103,-0.57
28622501\O,0,-1.7223737747,0.0637171932,-1.4971387833\O,0,-1.567708642
9,-1.3805311193,0.1278359827\\Version=EM64L-G09RevA.02\State=1-A\MP2/G
TBas1=-558.7258963\MP4/GTBas1=-558.8106967\CCSD (T) /G3Bas1=-558.7874119
\MP2/GTBas2=-558.7712374\MP4/GTBas2=-558.8598625\MP2/GTBas3=-559.10108
37\MP4/GTBas3=-559.2101967\HF/GTLargeXP=-557.395443\MP2/GTLargeXP=-559
.7899184\HF/GFHFB1=-557.4405753\HF/GFHFB2=-557.4499525\G4=-560.0316843
\FreqCoord=-0.1621952036,0.9196269473,0.3795327762,-0.9876150077,1.458
5222533,2.8203703796,2.1231021389,-1.0235668572,0.2209853017,0.5951083
504,3.0297867665,-1.000011759,-2.3560376861,-0.694769996,-0.8871860994
,0.3504182001,2.4076832753,3.8065958873,-1.506962615,-0.1346900283,3.7
480785219,3.0190143536,-1.7351647161,2.2045752931,2.793726156,-1.60046
62924,-1.9057534117,1.168146211,2.5419717978,-2.7613628862,-0.80101148
31,4.3366612791,-1.0825527645,-3.2548147327,0.1204080452,-2.8291822834
, -2.9625399912,-2.6088257335,0.2415749972\PG=C01 [X(C1H4N4O4)]\NImag=0
\\0.29659884,0.02935674,0.46336787,-0.08151330,-0.09447662,0.65533934,
-0.08231272,-0.02320352,0.02349996,0.37869997,-0.01797826,-0.10508422,
-0.02121169,0.27169853,0.55756247,0.07053074,-0.04215726,-0.26135465,0
.01965682,-0.01076442,0.64301980,-0.06536973,-0.00877040,0.00057144,-0
.01191598,0.01350063,0.00910818,0.45822287,-0.03012095,-0.07064410,0.0
0272874,0.01495877,-0.00522530,-0.00607584,-0.18563513,0.37736131,-0.0
0306590,0.00191753,-0.05483550,0.02186981,-0.01814305,-0.01891651,0.03
369579,-0.02322281,1.02274483,-0.08262564,0.00467361,0.031222116,-0.006
99693,-0.01544455,0.01903282,0.00812476,0.02645192,-0.01139502,0.40390
738,-0.03118251,-0.21259334,0.06988242,-0.00281974,0.01084165,0.002750
18,-0.00473489,-0.03621415,0.01221380,-0.21755489,0.56855119,0.0606605
5,0.09279963,-0.15353502,0.02308788,0.04168092,-0.03412199,-0.00390580
,0.00636095,-0.00033216,-0.17513291,-0.05373325,0.60681792,-0.06713635
,0.00579905,0.00679021,0.00873719,0.00732292,0.00175903,-0.03663130,0.
00215881,-0.01617469,-0.01011587,-0.01568154,-0.00297210,0.44300919,0.
02378050,-0.05946479,-0.00769000,-0.01017829,-0.01001045,-0.01557037,0
.00647977,0.03006699,0.01004516,-0.02532882,-0.02568763,0.00078789,0.1
0703376,0.67153501,0.01886742,-0.00666033,-0.06424234,-0.02491200,-0.0
2230353,-0.02715290,-0.01434621,0.00619939,0.01195168,0.00470762,0.013
37935,-0.00025267,0.16146012,-0.31238170,0.74378409,0.00589605,0.01214
341,0.01237212,-0.22739727,-0.17619380,-0.14881202,0.00084413,-0.00025
895,0.00292403,-0.00056301,0.00082329,0.00045782,0.00011762,-0.0013384
8,0.00187569,0.23026569,-0.00068531,-0.00623028,-0.01220192,-0.1384013
5,-0.12178857,-0.07801491,-0.00190622,0.00101543,-0.00345260,-0.000644
94,-0.00161637,0.00080358,-0.00246994,-0.00075456,0.00114585,0.1621524
0,0.14046192,-0.02978472,-0.02218660,-0.02443709,-0.12672821,-0.096922
07,-0.15780775,-0.00048782,0.00028485,-0.00048305,-0.00008806,0.000907
31,0.00331966,0.00613830,0.00144150,-0.00506312,0.14018899,0.10620333,

0.16988235,-0.01064843,-0.00664814,0.01415063,-0.04475003,-0.08047216,
 0.02991891,0.00213942,-0.00206111,0.00408129,0.00051956,0.00008788,0.0
 0076782,0.00138036,0.00403291,-0.00137464,-0.00841121,-0.02026517,0.01
 378809,0.05950163,0.00607292,0.00819650,-0.00235606,-0.11868563,-0.317
 10673,0.15698832,0.00067842,0.00049812,-0.00143284,0.00028235,0.000340
 45,-0.00245320,0.00106260,0.00319897,-0.00144361,0.00160102,-0.0136874
 1,0.01023148,0.10963308,0.32326627,0.00963248,0.03591743,-0.01960099,0
 .05171298,0.14166029,-0.14943292,-0.00012108,0.00032855,-0.00038230,0.
 00276281,-0.00350779,-0.00647654,0.00050195,0.00531521,-0.00442319,-0.
 00650312,-0.01833840,0.01228259,-0.05741657,-0.15933511,0.16175998,-0.
 00250980,0.01579734,-0.03101471,-0.00164842,0.00027095,0.00025028,-0.1
 9681656,0.10499179,-0.16820364,-0.00510002,0.00666598,0.00049321,-0.00
 086140,0.00688751,0.00219619,-0.00101097,0.00025847,0.00011743,0.00029
 153,0.00058989,-0.00020453,0.17060165,0.02319975,0.00644258,0.02520123
 ,0.00027647,-0.00146265,0.00004579,0.10419584,-0.14912070,0.13530130,0
 .00057611,-0.00157790,-0.00013528,-0.00036154,-0.01273582,-0.00055175,
 0.00016820,0.00055247,0.00023987,0.00061974,-0.00099102,-0.00002382,-0
 .11860321,0.11902723,-0.01007139,0.00596080,-0.01916108,0.00522873,-0.
 00375117,0.00914612,-0.17311143,0.13707467,-0.45545746,-0.00156467,0.0
 0217808,0.00189585,0.00146271,0.00700171,-0.00364664,-0.00064068,0.002
 28559,0.00106820,-0.00263648,-0.00009906,0.00102864,0.20063228,-0.1587
 7272,0.57619432,0.00616230,0.00647944,0.02809033,-0.00724933,0.0069281
 2,0.00533486,-0.16242897,0.07895351,0.14161568,-0.00061274,0.00404772,
 -0.00000262,0.00268701,0.00171292,0.00044152,-0.00043121,-0.00037150,-
 0.00029905,0.00093397,0.00028545,-0.00053402,0.03907614,-0.01287757,-0
 .01988083,0.12696902,0.01143989,0.00717964,-0.02188146,0.00681589,-0.0
 0461849,-0.00546903,0.07837720,-0.13315919,-0.11925066,0.00095843,-0.0
 0219455,0.00013762,-0.00122233,-0.00757261,-0.00141285,0.00027094,0.00
 055080,0.00039538,-0.00101727,-0.00029152,0.00022589,-0.01285227,0.033
 47478,0.01490808,-0.08596536,0.10181391,0.00874563,-0.00396764,-0.0193
 4476,0.00775939,-0.00587496,-0.00140795,0.14053048,-0.11756126,-0.4822
 3038,-0.00179311,0.00149698,0.00181697,-0.00081581,-0.00343184,-0.0051
 3002,-0.00076207,0.00221219,0.00053861,-0.00299766,-0.00000651,0.00041
 868,-0.00027261,-0.00316787,-0.11595518,-0.15397353,0.13276642,0.61059
 473,-0.01019228,-0.00581851,0.01361081,0.00059158,-0.00037796,0.000374
 43,0.00159486,-0.00197117,-0.00401366,-0.05246831,0.04064636,0.0873198
 3,0.00214332,-0.00120187,0.00433827,0.00005975,-0.00001667,0.00077206,
 0.00153095,-0.00004514,0.00022197,0.00007071,0.00079978,0.00110271,-0.
 00283074,0.00093637,0.00201273,0.06749159,-0.01258841,0.01094578,0.032
 65753,-0.00187664,-0.00599671,0.00300014,-0.00123675,0.00135924,0.0069
 0346,0.05353163,-0.08398040,-0.09380065,-0.00031511,-0.00054523,0.0015
 3260,0.00000367,-0.00006069,0.00000686,-0.00010802,0.00052890,0.001783
 79,-0.00030364,-0.00023599,-0.00262558,0.00145978,-0.00077115,-0.00410
 970,-0.04215660,0.08348500,0.00326512,-0.00599812,-0.02280622,0.001635
 73,0.00413898,-0.00021157,-0.00030881,0.00028703,-0.00279914,0.1287519
 8,-0.07684506,-0.37483723,-0.00050930,-0.00046111,0.00065741,0.0000874
 1,-0.00020647,0.00043568,0.00025773,-0.00057227,-0.00072320,0.00059352
 ,-0.00029468,0.00081135,0.00030839,-0.00183549,0.00162932,-0.12692797,
 0.08195069,0.39354997,0.00603570,-0.01589627,0.00042425,-0.00054792,-0
 .00096084,-0.00014025,0.00008916,-0.00029032,0.00225779,-0.24613251,0.
 22872774,0.01006993,0.00078905,-0.00171978,0.00215350,0.00005457,0.000
 63760,-0.00040726,0.00007414,-0.00005678,0.00006266,0.00031286,-0.0002
 9754,-0.00032011,0.00031114,0.00002312,-0.00060350,-0.00911994,0.00364
 505,-0.00610230,0.24957993,0.02265196,-0.03185089,0.00531526,0.0004762
 0,0.00157133,-0.00245238,-0.00241702,-0.00163800,0.00229721,0.18648036
 ,-0.20783641,0.01649425,0.00176055,-0.00128311,0.00282075,-0.00020096,
 0.00058748,-0.00014380,-0.00051824,0.00005038,-0.00014296,0.00084996,-

0.00065886,0.00065747,0.00014731,0.00054467,0.00002964,0.00495650,-0.00497823,0.00132914,-0.21419700,0.24155598,-0.02162171,0.01364413,0.00104501,0.00048340,-0.00255437,0.00011659,0.00613063,0.00220931,-0.00415204,-0.00089344,0.03569199,-0.05302324,0.00099135,-0.00103452,0.00187047,-0.00077957,0.00126919,-0.00063543,0.00058081,-0.00032544,0.00031005,-0.00241598,0.00041312,-0.00015430,-0.00108519,-0.00111150,0.00208970,0.02491194,-0.02591980,0.00428238,-0.00617536,-0.02384724,0.04947214,-0.00148166,0.00909289,-0.03303934,-0.00478635,-0.00537274,-0.00428735,-0.00052750,-0.00614442,-0.00293860,-0.00152520,-0.00045454,0.00017673,-0.19342584,0.03602071,-0.19604958,0.00028713,0.00106702,-0.00230340,0.00011997,-0.00014420,0.00068084,-0.00099574,0.00245193,-0.00039224,-0.00153269,0.00195270,0.00186790,0.00029199,-0.00025138,-0.00050527,-0.00099626,-0.00038017,-0.00013475,0.16704198,-0.01037982,0.00977364,0.00079328,0.00041310,0.00088902,-0.00080512,-0.00052564,-0.00549002,-0.00105825,-0.00382646,0.00155725,-0.00717504,0.03995246,-0.15558560,0.13966160,0.00044656,0.00018289,-0.00024945,-0.00125251,-0.00126000,-0.00161421,-0.00164103,0.00283258,-0.00170408,-0.00015917,0.00159208,0.00005766,0.00140613,-0.00003985,-0.00104176,0.00017197,0.00205656,0.00070530,-0.04924652,0.17387653,-0.02387564,0.02080741,-0.02352006,-0.00146702,-0.00309850,-0.00088216,0.00186984,-0.00850787,-0.01122559,0.00360038,-0.00316217,0.00600372,-0.19896244,0.13768467,-0.45238275,0.00001327,-0.00038057,-0.00097043,0.00018382,0.00071658,0.00178571,-0.00214211,0.00257875,0.00182376,0.00001812,0.00229609,0.00538953,-0.00228606,-0.00107478,0.00007657,-0.00052972,-0.00137003,-0.00045111,0.23038949,-0.21172713,0.52490102,0.00758371,-0.02300564,0.01483645,-0.00042379,-0.00292085,-0.00272644,0.00267483,-0.00103276,-0.00065289,-0.00641149,-0.00857085,-0.00102035,-0.15069299,-0.14618085,0.04064209,0.00028871,0.00064560,-0.00090634,-0.00268186,-0.00127397,-0.00079637,-0.00141000,-0.00014796,0.00019141,-0.00105390,0.00028270,0.00030216,0.00083651,0.00019642,-0.00054622,-0.00044992,0.00039054,0.00000786,0.03753016,0.02464093,-0.00681194,0.11421001,-0.01356650,-0.02003839,0.02323931,0.00052620,0.00042865,-0.00147511,0.00199417,-0.00880963,-0.00211827,-0.01015475,-0.00958979,-0.00176744,-0.14503969,-0.43116116,0.18001423,0.00038269,0.00078688,-0.00020866,-0.00203099,-0.00274290,-0.00226887,-0.00291174,0.00445331,-0.00311380,-0.00064065,0.00345162,0.00155689,0.00284278,0.00028933,-0.00045088,0.00021304,0.00187911,0.00085983,0.01140874,-0.03038508,0.06523756,0.15697668,0.49143806,-0.00176928,0.00439964,0.00645336,-0.00182747,-0.00285643,-0.00099410,0.00037478,-0.00010570,-0.00388237,0.00079045,-0.00125183,0.00272472,0.04033065,0.17829341,-0.19597000,-0.00042188,-0.00132485,0.00186977,0.00069627,0.00008773,0.00345349,-0.00002933,-0.00083395,0.00240642,-0.00003367,0.00023149,0.00159075,-0.00143706,-0.00030457,-0.00006530,-0.00068962,-0.00098730,-0.00077023,0.00653558,0.08415717,-0.05054821,-0.04251941,-0.25950480,0.23373171\\-0.00000210,0.00000532,0.00000304,0.00000240,-0.00000336,0.00000319,0.00000458,-0.00000670,-0.00000578,-0.00000148,0.00000019,-0.00000373,0.00000279,-0.000001525,-0.00000447,-0.00000351,-0.00000109,-0.00000813,-0.00000107,0.00000019,-0.00000021,-0.00000544,0.00000378,-0.00000102,-0.00000754,0.00000641,0.00000671,0.00000123,0.00000001,0.00000018,0.00000356,-0.00000608,0.00000491,0.00000178,0.00000443,0.00000408,0.00000481,0.00001214,0.00000123\\@

END OF SUPPORTING INFORMATION