Theoretical study of azido *gauche* effect and its origin

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Conformer	gas/CH_2Cl_2/DMSO/H_2O			
	ΔE	ΔH	ΔG	ΔG_{corr}
aaa, C_2	1.84/2.30/2.45/2.46	**1.91**/2.32/2.39/2.40	**1.79**/**2.19**/2.07/2.06	2.20/2.60/2.48/2.47
aag, C_1	1.80/2.11/2.22/2.23	1.97/2.22/2.27/2.27	2.06/2.20/**2.04**/**2.04**	**2.06**/**2.20**/**2.04**/**2.04**
gag, C_2	**1.70**/**1.85**/**1.91**/**1.92**	1.93/**2.05**/**2.04**/**2.04**	2.81/2.81/2.57/2.55	3.22/3.22/2.98/2.96
gag$^-$, C_i	1.76/1.91/1.99/2.01	2.01/2.11/2.11/2.11	2.47/2.47/2.26/2.24	2.88/2.88/2.67/2.65
aga, C_2	1.49/1.13/1.06/1.05	1.61/1.13/0.99/0.97	1.90/0.90/0.86/0.86	2.31/1.31/1.27/1.27
agg, C_1	1.74/1.12/1.01/1.00	1.88/1.21/1.04/1.02	2.11/1.34/1.00/0.98	2.11/1.34/1.00/0.98
ag$^-$*g*, C_1	0.13/0.10/0.14/0.15	0.22/0.14/0.12/0.12	0.39/**0.00**/**0.00**/**0.00**	0.39/**0.00**/**0.00**/**0.00**
ggg, C_2	1.44/0.99/0.93/0.92	1.65/1.18/1.04/1.03	2.61/1.86/1.48/1.45	3.02/2.27/1.90/1.86
gg$^-$*g*, C_1	**0.00**/**0.00**/0.04/0.05	**0.00**/**0.00**/**0.00**/**0.00**	**0.00**/0.31/0.29/0.29	**0.00**/0.31/0.29/0.29
ggg$^-$, C_1	0.26/0.02/**0.00**/**0.00**	0.42/0.12/0.03/0.02	1.32/0.83/0.55/0.53	1.32/0.83/0.55/0.53
Isomerization	ΔΔE	ΔΔH	ΔΔG	$\Delta\Delta G_{corr}$
aaa → *aga*	-0.35/-1.18/-1.38/-1.41	-0.30/-1.19/-1.40/-1.42	0.11/-1.29/-1.21/-1.20	0.11/-1.29/-1.21/-1.20
aag → *agg*	-0.06/-0.98/-1.20/-1.23	-0.09/-1.01/-1.23/-1.25	0.05/-0.86/-1.04/-1.06	0.05/-0.86/-1.04/-1.06
aag → *ag*$^-$*g*	-1.67/-2.01/-2.07/-2.08	-1.75/-2.09/-2.15/-2.16	-1.67/-2.20/-2.04/-2.04	-1.67/-2.20/-2.04/-2.04
gag → *ggg*	-0.26/-0.85/-0.99/-1.00	-0.28/-0.87/-1.00/-1.01	-0.21/-0.95/-1.08/-1.10	-0.21/-0.95/-1.08/-1.10
gag → *gg*$^-$*g*	-1.70/-1.85/-1.87/-1.87	-1.93/-2.05/-2.04/-2.04	-2.81/-2.50/-2.28/-2.26	-3.22/-2.91/-2.69/-2.67
gag$^-$ → *ggg*$^-$	-1.50/-1.89/-1.99/-2.01	-1.60/-1.99/-2.09/-2.10	-1.15/-1.64/-1.71/-1.71	-1.56/-2.05/-2.12/-2.12
anti → *gauche*[a]	**-1.70**/**-1.85**/**-1.91**/**-1.92**	**-1.91**/**-2.05**/**-2.04**/**-2.04**	**-1.79**/**-2.19**/**-2.04**/**-2.04**	**-2.06**/**-2.20**/**-2.04**/**-2.04**

[a] Energy difference between the most stable CC_{gauche} and the most stable CC_{anti} conformer (bolded numbers for each energy term).

Table S2. Contribution of various energy components to the total binding interactions between two $N_3CH_2\cdot$ fragments in diazidoethane and energy changes (ΔΔE values) occuring upon conformational isomerization.[a] Data for 1,2-difluoroethane (DFE) are included for comparison.[b] Values are in kcal/mol, obtained at the MP2/6-311++G(d,p) level.

Conformer	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{Pauli}
aaa	-115.76	33.19	-148.95	-147.21	-151.59	-66.53	216.38
aag	-115.92	25.41	-141.33	-150.53	-153.35	-67.77	230.32
gag	-116.08	17.39	-133.47	-153.37	-154.27	-68.61	242.78
	-117.06	*16.10*	*-133.13*	*-146.20*	*-159.90*	*-67.73*	*240.70*
gag$^-$	-116.01	17.21	-133.22	-153.73	-154.59	-68.20	243.30
aga	-116.22	21.64	-137.86	-147.87	-154.09	-55.86	219.96
agg	-115.98	20.16	-136.14	-150.40	-154.47	-62.10	230.83
ag$^-$*g*	-117.53	24.57	-142.10	-153.13	-156.05	-68.37	235.45
ggg	-116.29	18.59	-134.88	-154.48	-154.14	-68.09	241.83
gg$^-$*g*	-117.62	17.57	-135.19	-153.92	-157.16	-71.50	247.39
	-118.88	*17.29*	*-136.19*	*-148.16*	*-163.12*	*-71.24*	*246.33*
ggg$^-$	-117.46	17.95	-135.41	-155.45	-155.91	-70.93	246.88
a DFE	-97.82	10.31	-108.13	-148.82	-155.48	-25.50	221.67
g DFE	-98.58	10.50	-109.08	-152.20	-160.01	-26.11	229.24
Isomerization	ΔE_{iso}	$\Delta\Delta E_{def}$	$\Delta\Delta E_{int}$	$\Delta\Delta E_{elstat}$	$\Delta\Delta E_{oi}$	$\Delta\Delta E_{disp}$	$\Delta\Delta E_{Pauli}$
aaa → *aga*	-0.35	-11.44	11.09	-0.66	-2.50	10.67	3.58
				(20.9)	(79.1)		
aag → *agg*	-0.06	-5.25	5.19	0.13	-1.12	5.67	0.51
aag → *ag*$^-$*g*	-1.67	-0.90	-0.77	-2.60	-2.70	-0.60	5.13
				(44.1)	(45.8)	(10.1)	
gag → *ggg*	-0.26	1.15	-1.41	-1.11	-0.13	0.52	-0.95
				(50.7)	(5.9)		(43.4)
gag → *gg*$^-$*g*[c]	-1.70	0.02	-1.72	-0.55	-2.89	-2.89	4.61
				(8.6)	(45.7)	(45.7)	
	-1.87	*1.19*	*-3.06*	*-1.96*	*-3.22*	*-3.51*	*5.63*
				(22.6)	*(37.1)*	*(40.3)*	
gag$^-$ → *ggg*$^-$	-1.50	0.69	-2.19	-1.72	-1.32	-2.73	3.58
				(29.8)	(22.9)	(47.3)	
a DFE → *g* DFE	-0.77	0.18	-0.95	-3.38	-4.53	-0.61	7.57
				(39.7)	(53.2)	(7.1)	

[a] ΔE_{tot} = total binding energy between two radical fragments, ΔE_{def} = deformation energy, ΔE_{int} = interaction energy, ΔE_{elstat} = electrostatic energy, ΔE_{oi} = orbital interaction energy, ΔE_{disp} = dispersion energy, ΔE_{Pauli} = Pauli repulsion, ΔE_{iso} = isomerization energy, ΔΔE values represent individual energy changes upon conformational isomerization. Values in italic are in H_2O. Values in parentheses are percentage contribution to all attractive interactions contained in $\Delta\Delta E_{int}$. [b]From ref. 3f. [c]Corresponds to the most stable CC_{anti} → the most stable CC_{gauche} isomerization.

Table S3. Energies of vicinal hyperconjugative interactions between two N_3CH_2 fragments in 1,2-diazidoethane and their change upon conformational isomerization, estimated on the basis of second-order perturbative approach at the HF/6-311++G(d,p) level.[a] Energies are in kcal/mol.

Conformer	total	$total_{gauche}$	$total_{anti}$	$\sigma_{CH} \rightarrow \sigma^*_{CH}$	$\sigma_{CN} \rightarrow \sigma^*_{CN}$	$\sigma_{CH} \rightarrow \sigma^*_{CN}$	$\sigma_{CN} \rightarrow \sigma^*_{CH}$
aag, C_1	-20.27	-3.92	-16.35	-3.19/-2.90/-3.12/-3.28	-2.09/-1.77		
gag, C_2	-20.06	-3.74	-16.32	-3.34/-2.82/-2.82/-3.34	-2.00/-2.00		
gag$^-$, C_i	-19.98	-3.76	-16.22	-3.01/-3.14/-3.01/-3.14	-1.96/-1.96		
ag$^-$*g*, C_1	-21.46	-3.94	-17.52	-3.29/-3.27		-3.88/-4.37	-1.38/-1.33
ggg$^-$, C_1	-21.69	-3.69	-18.00	-3.49/-2.97		-4.32/-4.59	-1.25/-1.38
gg$^-$*g*, C_1	-21.62	-3.69	-18.93	-3.28/-3.23		-4.47/-4.51	-1.21/-1.23
Isomerization							
aag $\rightarrow$ *ag*$^-$*g*	-1.19	-0.02	-1.17				
gag $\rightarrow$ *gg*$^-$*g*	-1.56	0.05	-1.61				
gag$^-$ $\rightarrow$ *ggg*$^-$	-1.71	0.07	-1.78				

[a] Individual interactions correspond to *anti* vicinal hyperconjugation. $Total_{anti}$ is the sum of six interactions between *anti*-related σ-bonds. $Total_{gauche}$ is the sum of twelve interactions between *gauche*-related σ-bonds. Total is the sum of all vicinal hyperconjugations, that is $total_{anti} + total_{gauche}$.

Table S4. Relative energies (ΔE), enthalpies (ΔH), free energies (ΔG), free energies corrected for ΔS_{sym} and ΔS_{mix} (ΔG_{corr}) for fourteen conformers of 2-azidoethanamine in the gas-phase and in solvents (CH_2Cl_2, DMSO and H_2O) and energy changes (ΔΔ values) upon conformational isomerizations, obtained at the MP2/6-311++G(d,p) level. All values are in kcal/mol.

Conformer	gas/CH_2Cl_2/DMSO/H_2O			
	ΔE	ΔH	ΔG	ΔG_{corr}
aaa, C_s	1.93/1.19/1.14/1.14	1.87/1.16/1.11/1.11	**1.16**/**0.69**/**0.52**/**0.50**	1.57/**1.10**/**0.93**/**0.91**
aag, C_1	1.67/1.41/1.48/1.49	1.69/1.39/1.45/1.46	1.49/1.24/1.16/1.16	**1.49**/1.24/1.16/1.16
gaa, C_1	1.63/**0.86**/**0.82**/**0.82**	1.71/**0.93**/**0.89**/**0.89**	1.95/1.26/1.09/1.08	1.95/1.26/1.09/1.08
gag, C_1	**1.49**/1.16/1.23/1.23	**1.61**/1.21/1.28/1.29	1.75/1.40/1.36/1.36	1.75/1.40/1.36/1.36
gag$^-$, C_1	1.53/1.20/1.25/1.26	1.62/1.23/1.27/1.28	1.75/1.40/1.33/1.32	1.75/1.40/1.33/1.32
aga, C_1	0.51/0.13/0.16/0.16	0.43/0.07/0.10/0.10	0.10/0.09/0.11/0.12	0.10/0.09/0.11/0.12
agg, C_1	**0.00**/0.10/0.23/0.24	**0.00**/0.04/0.16/0.17	**0.00**/**0.00**/**0.00**/**0.00**	**0.00**/**0.00**/**0.00**/**0.00**
ag$^-$*g*, C_1	- /- /1.44/1.41	- /- /1.31/1.28	- /- /0.90/0.83	- /- /0.90/0.83
gga, C_1	0.70/0.10/0.10/0.11	0.74/0.16/0.17/0.17	1.12/0.73/0.65/0.65	1.12/0.73/0.65/0.65
ggg, C_1	0.32/0.14/0.19/0.20	0.40/0.19/0.23/0.24	0.85/0.74/0.68/0.68	0.85/0.74/0.68/0.68
ggg$^-$, C_1	1.99/1.04/0.90/0.88	2.03/1.09/0.94/0.93	2.33/1.10/1.05/1.04	2.33/1.10/1.05/1.04
gg$^-$*a*, C_1	0.99/0.50/0.51/0.51	1.00/0.50/0.51/0.51	1.42/0.94/0.83/0.82	1.42/0.94/0.83/0.82
gg$^-$*g*$^-$, C_1	0.52/0.38/0.46/0.47	0.57/0.39/0.49/0.50	0.80/0.84/0.87/0.88	0.80/0.84/0.87/0.88
gg$^-$*g*, C_1	0.48/**0.00**/**0.00**/**0.00**	0.47/**0.00**/**0.00**/**0.00**	1.02/0.65/0.57/0.56	1.02/0.65/0.57/0.56
Isomerization	ΔΔE	ΔΔH	ΔΔG	$\Delta\Delta G_{corr}$
aaa → *aga*	-1.42/-1.06/-0.99/-0.98	-1.44/-1.10/-1.01/-1.00	-1.07/-0.60/-0.40/-0.39	-1.48/-1.01/-0.81/-0.80
aag → *agg*	-1.67/-1.31/-1.25/-1.24	-1.69/-1.35/-1.30/-1.29	-1.49/-1.24/-1.16/-1.16	-1.49/-1.24/-1.16/-1.16
aag → *ag*$^-$*g*	- /- /-0.04/-0.08	- /- /-0.14/-0.18	- /- /-0.27/-0.33	- /- /-0.27/-0.33
gaa → *gga*	-0.93/-0.76/-0.72/-0.71	-0.96/-0.77/-0.72/-0.71	-0.83/-0.52/-0.44/-0.43	-0.83/-0.52/-0.44/-0.43
gaa → *gg*$^-$*a*	-0.64/-0.36/-0.31/-0.31	-0.70/-0.44/-0.38/-0.38	-0.52/-0.32/-0.27/-0.26	-0.52/-0.32/-0.27/-0.26
gag → *ggg*	-1.17/-1.02/-1.03/-1.04	-1.21/-1.03/-1.04/-1.05	-0.89/-0.66/-0.68/-0.68	-0.89/-0.66/-0.68/-0.68
gag → *gg*$^-$*g*	-1.01/-1.16/-1.23/-1.23	-1.13/-1.21/-1.28/-1.29	-0.72/-0.75/-0.80/-0.80	-0.72/-0.75/-0.80/-0.80
gag$^-$ → *ggg*$^-$	0.46/-0.16/-0.35/-0.37	0.42/-0.14/-0.33/-0.35	0.58/-0.30/-0.27/-0.28	0.58/-0.30/-0.27/-0.28
gag$^-$ → *gg*$^-$*g*$^-$	-1.01/-0.82/-0.79/-0.78	-1.04/-0.83/-0.78/-0.77	-0.95/-0.56/-0.45/-0.44	-0.95/-0.56/-0.45/-0.44
anti → *gauche*[a]	**-1.49/-0.86/-0.82/-0.82**	**-1.61/-0.93/-0.89/-0.89**	**-1.16/-0.69/-0.52/-0.50**	**-1.49/-1.10/-0.93/-0.91**

[a] Energy difference between the most stable CC_{gauche} and the most stable CC_{anti} conformer (bolded numbers for each energy term).

Table S5. Contribution of various energy components to the total binding interactions between $N_3CH_2\cdot$ and $\cdot CH_2NH_2$ fragments and energy changes (ΔΔE values) occuring upon conformational isomerization.[a] Data for 2-fluoroethanamine (2FEA) are included for comparison.[b] Values are in kcal/mol, obtained at the MP2/6-311++G(d,p) level.

Conformer	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{Pauli}
aaa	-99.45	23.92	-123.37	-158.94	-155.77	-47.67	239.01
aag	-99.69	29.87	-129.56	-153.75	-153.18	-49.03	226.40
gaa	-99.78	15.13	-114.91	-162.24	-156.85	-47.46	251.64
	-99.17	*15.04*	*-114.11*	*-155.81*	*-164.73*	*-47.07*	*253.50*
gag	-99.93	21.82	-121.75	-157.03	-154.38	-49.50	239.16
gag$^-$	-99.89	21.91	-121.80	-156.98	-154.52	-49.70	239.40
aga	-100.86	23.91	-124.77	-160.90	-156.25	-47.93	240.31
agg	-101.36	30.90	-132.26	-155.00	154.29	-50.14	227.17
gga	-100.72	15.51	-116.23	-164.30	-157.49	-47.95	253.51
ggg	-101.11	23.84	-124.95	-157.96	-155.12	-51.24	239.37
ggg$^-$	-99.41	24.02	-123.43	-155.86	-153.49	-48.59	234.51
gg$^-$*a*	-100.38	15.36	-115.74	-162.98	-158.73	-48.78	254.75
	-99.81	*15.57*	*-114.95*	*-157.05*	*-166.12*	*-48.33*	*256.55*
gg$^-$*g*$^-$	-100.87	21.08	-121.95	-159.28	-157.59	-50.41	245.33
gg$^-$*g*	-100.88	21.45	-122.33	-160.09	-156.78	-50.72	245.26
	-99.74	*21.46*	*-121.35*	*-153.94*	*-163.32*	*-50.71*	*246.62*
ag 2FEA	-90.92	17.74	-108.66	-155.31	-155.91	-27.54	230.10
gg 2FEA	-92.31	19.67	-111.98	-156.77	-157.53	-28.82	231.14
Isomerization	ΔE_{iso}	$\Delta\Delta E_{def}$	$\Delta\Delta E_{int}$	$\Delta\Delta E_{elstat}$	$\Delta\Delta E_{oi}$	$\Delta\Delta E_{disp}$	$\Delta\Delta E_{Pauli}$
aaa → *aga*	-1.42	-0.02	-1.40	-1.96	-0.48	-0.26	1.30
				(72.6)	(17.8)	(9.6)	
aag → *agg*	-1.67	1.03	-2.70	-1.25	-1.11	-1.11	0.77
				(36.0)	(32.0)	(32.0)	
gaa → *gga*	-0.93	0.39	-1.32	-2.06	-0.64	-0.49	1.87
				(64.6)	(20.1)	(15.3)	
gaa → *gg*$^-$*a*	-0.64	0.19	-0.83	-0.74	-1.88	-1.32	3.11
				(18.8)	(47.7)	(33.5)	
gag → *ggg*	-1.17	2.03	-3.20	-0.93	-0.74	-1.74	0.21
				(27.3)	(21.7)	(51.0)	
gag → *gg*$^-$*g*	-1.01	-0.43	-0.58	-3.06	-2.40	-1.22	6.10
				(45.8)	(35.9)	(18.3)	
gag$^-$ → *ggg*$^-$	0.46	2.09	-1.63	1.12	1.03	1.11	-4.89
gag$^-$ → *gg*$^-$*g*$^-$	-1.01	-0.86	-0.15	-2.30	-3.07	-0.71	5.93
				(37.8)	(50.5)	(11.7)	
gag → *ggg*	-1.17	2.03	-3.20	-0.93	-0.74	-1.74	0.21
ggg → *agg*	-0.32	6.99	-7.31	2.96	0.83	1.10	-12.20
gag → *agg*[c]	-1.49	9.02	-10.51	2.03	0.09	-0.64	-11.99

gag → *aag*	0.18	7.99	-7.81	3.28	1.20	0.47	-12.76
aag → *agg*	-1.67	1.03	-2.70	-1.25	-1.11	-1.11	0.77
gag → *agg*[c]	-1.49	9.02	-10.51	2.03	0.09	-0.64	-11.99
gaa → *gg*$^{-}$*a*	*-0.31*	*0.53*	*-0.84*	*-1.24*	*-1.39*	*-1.26*	*3.05*
				(31.9)	*(35.7)*	*(32.4)*	
gg^{-}*a* → *gg*$^{-}$*g*	*-0.51*	*5.89*	*-6.40*	*3.11*	*2.80*	*-2.38*	*-9.93*
						(19.3)	*(80.7)*
gaa → *gg*$^{-}$*g*[c]	*-0.82*	*6.42*	*-7.24*	*1.87*	*1.41*	*-3.64*	*-6.88*
ag 2FEA → *gg* 2FEA	-1.40	1.92	-3.32	-1.46	-1.62	-1.28	1.04
				(33.5)	(37.2)	(29.3)	

[a] Labeling of various energy terms is the same as in Table 2. Values in italic are in H_2O. Values in parentheses are percentage contribution to all attractive interactions. [b]From ref. 3f. [c]Corresponds to the most stable CC_{anti} → the most stable CC_{gauche} isomerization.

Table S6. Energies of vicinal hyperconjugative interactions between N_3CH_2 and CH_2NH_2 fragments in 2-azidoethanamine and their change upon conformational isomerization, estimated on the basis of second-order perturbative approach at the HF/6-311++G(d,p) level.[a] Energies are in kcal/mol.

Conformer	total	$total_{gauche}$	$total_{anti}$	$\sigma_{CH} \rightarrow \sigma^*_{CH}$	$\sigma_{CN3} \rightarrow \sigma^*_{CNH2}$/ $\sigma_{CNH2} \rightarrow \sigma^*_{CN3}$	$\sigma_{CH} \rightarrow \sigma^*_{CN3}$/ $\sigma_{CH} \rightarrow \sigma^*_{CNH2}$	$\sigma_{CN3} \rightarrow \sigma^*_{CH}$/ $\sigma_{CNH2} \rightarrow \sigma^*_{CH}$
aaa	-20.63	-3.34	-17.29	-3.63/-3.63/-3.01/-3.01	-2.26/-1.75		
aag	-20.66	-3.65	-17.01	-3.32/-3.63/-3.00/-3.00	-1.90/-2.16		
gaa	-20.28	-3.21	-17.07	-3.63/-3.32/-2.96/-3.11	-2.10/-1.95		
gag	-20.46	-3.50	-16.96	-3.33/-3.37/-2.99/-3.09	-1.79/-2.39		
gag$^-$	-20.57	-3.55	-17.02	-3.69/-3.03/-2.95/-3.14	-1.82/-2.39		
aga	-21.74	-3.28	-18.46	-3.81/-3.02		-4.34/-4.76	-1.27/-1.26
agg	-21.69	-3.70	-17.99	-3.56/-3.10		-4.42/-3.98	-1.34/-1.59
gga	-22.09	-3.13	-18.96	-3.54/-3.18		-5.00/-4.73	-1.25/-1.26
ggg	-22.08	-3.60	-18.48	-3.32/-3.22		-5.09/-3.94	-1.32/-1.59
gg$^-$*a*	-22.27	-3.14	-19.13	-3.84/-3.01		-5.10/-4.98	-1.15/-1.05
gg$^-$*g*$^-$	-21.60	-3.36	-18.24	-3.52/-3.05		-4.86/-4.07	-1.30/-1.44
gg$^-$*g*	-21.70	-3.56	-18.14	-3.75/-3.05		-4.55/-4.13	-1.27/-1.39
Isomerization							
aaa → *aga*	-1.11	0.06	-1.17				
aag → *agg*	-1.03	-0.05	-0.98				
gaa → *gga*	-1.81	0.08	-1.89				
gaa → *gg*$^-$*a*	-1.99	0.07	-2.06				
gag → *ggg*	-1.62	-0.10	-1.52				
gag → *gg*$^-$*g*	-1.24	-0.06	-1.18				
gag$^-$ → *gg*$^-$*g*$^-$	-1.03	0.19	-1.22				

[a] Individual interactions correspond to *anti* vicinal hyperconjugation. $Total_{anti}$ is the sum of six interactions between *anti*-related σ-bonds. $Total_{gauche}$ is the sum of twelve interactions between *gauche*-related σ-bonds. Total is the sum of all vicinal hyperconjugations, that is $total_{anti} + total_{gauche}$.

Table S7. Relative energies (ΔE), enthalpies (ΔH) and free energies (ΔG) for four conformers of 2-azidoethylammonium cation in the gas-phase and in solvents (CH_2Cl_2, DMSO and H_2O) and energy changes (ΔΔ values) upon conformational isomerizations, obtained at the MP2/6-311++G(d,p) level. All values are in kcal/mol.

Conformer	gas/CH_2Cl_2/DMSO/H_2O		
	ΔE	ΔH	ΔG
aa, C_1	**8.60/3.58/2.97/2.91**	**8.60/3.83/3.21/3.14**	**7.57/3.24/3.11/3.08**
ag, C_1	9.79/3.80/3.05/2.98	9.77/4.19/3.41/3.33	9.00/4.46/3.83/3.77
ga, C_1	**0.00/0.00/0.00/0.00**	**0.00/0.00/0.00/0.00**	**0.00/0.00/0.00/0.00**
gg, C_1	- /0.83/0.59/0.57	- /0.83/0.66/0.63	- /1.08/1.31/1.32
Isomerization	ΔΔE	ΔΔH	ΔΔG
aa → *ga*[a]	**-8.60/-3.58/-2.97/-2.91**	**-8.60/-3.38/-3.21/-3.14**	**-7.57/-3.24/-3.11/-3.08**
ag → *gg*	- /-2.97/-2.46/-2.41	- /-3.36/-2.75/-2.70	- /-3.38/-2.52/-2.45

[a] Energy difference between the most stable CC_{gauche} and the most stable CC_{anti} conformer (bolded numbers for each energy term).

Table S8. Contribution of various energy components to the total binding interactions between $N_3CH_2\cdot$ and $\cdot CH_2NH_3^+$ fragments in the most stable CC_{anti} and the most stable CC_{gauche} forms and energy changes (ΔΔE values) occuring upon conformational isomerization.[a] Data for 2-fluoroethylammonium cation (2FEAH) are included for comparison.[b] Values are in kcal/mol, obtained at the MP2/6-311++G(d,p) level.

Conformer	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{Pauli}
aa	-110.10	21.79	-131.89	-133.27	-153.87	-47.32	202.57
	-107.74	*20.69*	*-128.43*	*-64.82*	*-223.85*	*-47.89*	*208.13*
ga	-118.66	21.05	-139.71	-143.77	-158.52	-47.05	209.63
	-110.65	*20.35*	*-131.00*	*-75.03*	*-221.53*	*-48.20*	*213.76*
a FEAH	-99.18	11.22	-110.40	-131.03	-151.97	-29.64	202.24
g FEAH	-106.02	11.56	-117.58	-140.48	-155.52	-29.78	208.20
Isomerization	ΔE_{iso}	$\Delta\Delta E_{def}$	$\Delta\Delta E_{int}$	$\Delta\Delta E_{elstat}$	$\Delta\Delta E_{oi}$	$\Delta\Delta E_{disp}$	$\Delta\Delta E_{Pauli}$
aa → *ga*	-8.57	-0.75	-7.82	-10.50 (69.3)	-4.65 (30.7)	0.27	7.06
	-2.91	*-0.34*	*-2.57*	*-10.21 (97.1)*	*2.32*	*-0.31 (2.9)*	*5.63*
a 2FEAH → *g* 2FEAH	-6.84	0.34	-7.18	-9.45 (71.9)	-3.55 (27.0)	-0.14 (1.1)	5.96

[a] Labeling of various energy terms is the same as in Table 2. Values in italic are in H_2O. Values in parentheses are percentage contribution to all attractive interactions. [b]From ref. 3f.

Table S9. Energies of vicinal hyperconjugative interactions between N_3CH_2 and $CH_2NH_3^+$ fragments in the most stable CC_{anti} and the most stable CC_{gauche} isomer of 2-azidoethylammonium cation and their changes upon conformational isomerization, estimated on the basis of second-order perturbative approach at the HF/6-311++G(d,p) level.[a] Energies are in kcal/mol.

Conformer	total	$total_{gauche}$	$total_{anti}$	$\sigma_{CH} \rightarrow \sigma^*_{CH}$	$\sigma_{CN3} \rightarrow \sigma^*_{CNH3}$/ $\sigma_{CNH3} \rightarrow \sigma^*_{CN3}$	$\sigma_{CH} \rightarrow \sigma^*_{CN3}$/ $\sigma_{CH} \rightarrow \sigma^*_{CNH3}$	$\sigma_{CN3} \rightarrow \sigma^*_{CH}$/ $\sigma_{CNH3} \rightarrow \sigma^*_{CH}$
aa	-20.47	-4.02	-16.45	-2.83/-2.80/-3.04/-3.05	-3.55/-1.18		
	-20.14	*-4.05*	*-16.09*	*-2.90/-2.91/-2.97/-2.93*	*-2.84/-1.54*		
ga	-20.48	-3.99	-16.49	-2.86/-2.96		-2.60/-5.34	-1.58/-1.15
	-21.68	*-3.98*	*-17.70*	*-3.07/-3.05*		*-3.52/-5.49*	*-1.37/-1.20*
Isomerization							
aa → *ga*	-0.01	0.03	-0.04				
	-1.54	*0.07*	*-1.61*				

[a] Individual interactions correspond to *anti* vicinal hyperconjugation. $Total_{anti}$ is the sum of six interactions between *anti*-related σ-bonds. $Total_{gauche}$ is the sum of twelve interactions between *gauche*-related σ-bonds. Total is the sum of all vicinal hyperconjugations, that is $total_{anti} + total_{gauche}$. Values in italic are from H_2O.

Table S10. Relative energies (ΔE), enthalpies (ΔH) and free energies (ΔG) for fourteen conformers of 2-azidoethanol in the gas-phase and in solvents (CH_2Cl_2, DMSO and H_2O) and energy changes (ΔΔ values) upon conformational isomerizations, obtained at the MP2/6-311++G(d,p) level. All values are in kcal/mol.

Conformer	gas/CH_2Cl_2/DMSO/H_2O		
	ΔE	ΔH	ΔG
aaa, C_1	2.49/2.23/2.24/2.25	2.36/2.13/2.19/2.20	**1.24**/**1.13**/**1.20**/**1.20**
aag, C_1	2.82/2.13/2.04/2.04	2.81/2.21/2.16/2.15	2.44/1.78/1.62/1.60
gaa, C_1	**2.39**/2.03/2.03/2.04	**2.36**/**2.01**/2.06/2.06	1.97/1.59/1.48/1.47
gag, C_1	2.75/1.96/**1.85**/**1.84**	2.81/2.03/**1.96**/**1.96**	2.82/2.01/1.84/1.82
gag$^-$, C_1	2.69/**1.93**/1.85/1.85	2.77/2.08/2.03/2.03	2.78/2.13/1.95/1.93
aga, C_1	- /1.44/1.22/1.20	- /1.30/1.11/1.09	- /0.76/0.37/0.35
agg, C_1	3.44/1.67/1.32/1.29	3.32/1.63/1.32/1.29	2.98/1.41/0.88/0.82
ag$^-$*g*, C_1	**0.00**/**0.00**/0.05/0.07	**0.00**/**0.00**/0.09/0.10	**0.00**/**0.00**/**0.00**/**0.00**
gga, C_1	2.76/1.45/1.21/1.19	2.67/1.38/1.19/1.17	2.44/1.17/0.91/0.88
ggg, C_1	2.69/1.33/1.08/1.06	2.72/1.43/1.22/1.20	2.84/1.53/1.26/1.22
ggg$^-$, C_1	0.60/0.32/0.30/0.31	0.68/0.41/0.43/0.43	1.05/0.83/0.74/0.73
gg$^-$*a*, C_1	0.70/0.06/**0.00**/**0.00**	0.63/0.01/**0.00**/**0.00**	0.83/0.17/0.08/0.07
gg$^-$*g*$^-$, C_1	1.58/0.35/0.12/0.11	1.56/0.42/0.23/0.21	1.94/0.88/0.60/0.57
gg$^-$*g*, C_1	1.41/- /- /-	1.29/- /- /-	0.96/- /- /-
Isomerization	ΔΔE	ΔΔH	ΔΔG
aaa → *aga*	- /-0.79/-1.02/-1.05	- /-0.83/-1.08/-1.11	- /-0.37/-0.83/-0.85
aag → *agg*	0.62/-0.46/-0.72/-0.75	0.51/-0.58/-0.84/-0.87	0.54/-0.37/-0.74/-0.78
aag → *ag*$^-$*g*	-2.82/-2.13/-1.99/-1.97	-2.81/-2.21/-2.07/-2.05	-2.44/-1.78/-1.62/-1.60
gaa → *gga*	0.37/-0.58/-0.82/-0.85	0.32/-0.63/-0.87/-0.90	0.47/-0.42/-0.56/-0.59
gaa → *gg*$^-$*a*	-1.69/-1.98/-2.03/-2.04	-1.73/-2.00/-2.06/-2.06	-1.14/-1.42/-1.40/-1.40
gag → *ggg*	-0.06/-0.63/-0.77/-0.79	-0.09/-0.61/-0.74/-0.76	0.02/-0.48/-0.58/-0.60
gag → *gg*$^-$*g*	-1.34/- /- /-	-1.52/- /- /-	-1.86/- /- /-
gag$^-$ → *ggg*$^-$	-2.09/-1.61/-1.55/-1.54	-2.10/-1.66/-1.60/-1.59	-1.73/-1.29/-1.21/-1.20
gag$^-$ → *gg*$^-$*g*$^-$	-1.11/-1.59/-1.73/-1.74	-1.22/-1.66/-1.80/-1.81	-0.84/-1.24/-1.34/-1.35
anti → *gauche*[a]	**-2.39**/**-1.93**/**-1.85**/**-1.84**	**-2.36**/**-2.01**/**-1.96**/**-1.96**	**-1.24**/**-1.13**/**-1.20**/**-1.20**

[a] Energy difference between the most stable CC_{gauche} and the most stable CC_{anti} conformer (bolded numbers for each energy term).

Table S11. Contribution of various energy components to the total binding interactions between $N_3CH_2\cdot$ and $\cdot CH_2OH$ fragments and energy changes (ΔΔE values) occuring upon conformational isomerization.[a] Data for 2-fluoroethanol (2FE) are included for comparison.[b] Values are in kcal/mol, obtained at the MP2/6-311++G(d,p) level.

Conformer	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{Pauli}
aag	-102.68	22.06	-124.74	-154.60	-154.83	-46.05	230.74
gaa	-103.13	20.91	-124.04	-153.63	-154.67	-49.63	233.89
gag	-102.77	14.61	-117.38	-157.64	-156.44	-47.42	244.12
	-102.67	*14.21*	*-116.90*	*-148.73*	*-164.13*	*-47.21*	*243.17*
gag⁻	-102.83	14.43	-117.26	-157.96	-156.42	-47.09	244.21
agg	-102.06	21.59	-123.65	-154.16	-156.39	-45.59	232.49
ag⁻g	-105.47	22.07	-127.54	-158.96	-156.96	-46.57	234.95
gga	-102.73	21.39	-124.12	-154.35	-155.94	-49.46	235.63
ggg	-102.84	15.92	-118.76	-158.62	-156.52	-46.94	243.32
ggg⁻	-104.95	15.26	-120.21	-162.16	-158.35	-48.23	248.53
gg⁻a	-104.76	20.63	-125.39	-157.12	-157.53	-50.37	239.63
	-104.55	*20.25*	*-124.78*	*-149.74*	*-164.32*	*-50.58*	*239.86*
gg⁻g⁻	-103.91	14.55	-118.46	-160.83	-158.91	-48.09	249.37
gg⁻g	-104.07	14.41	-118.48	-160.49	-159.36	-47.79	249.16
ag⁻ 2FE	-93.76	10.91	-104.67	-155.52	-157.32	-25.64	233.81
gg⁻ 2FE	-96.30	11.48	-107.78	-160.86	-160.35	-26.15	239.58
Isomerization	ΔE_{iso}	$\Delta\Delta E_{def}$	$\Delta\Delta E_{int}$	$\Delta\Delta E_{elstat}$	$\Delta\Delta E_{oi}$	$\Delta\Delta E_{disp}$	$\Delta\Delta E_{Pauli}$
aag → *agg*	0.62	-0.47	1.09	0.44	-1.56	0.46	1.75
aag → *ag⁻g*	-2.82	-0.02	-2.80	-4.36	-2.13	-0.52	4.21
				(62.2)	(30.4)	(7.4)	
gaa → *gga*	0.37	0.45	-0.08	-0.72	-1.27	0.17	1.74
				(36.2)	(63.8)		
gaa → *gg⁻a*	-1.69	-0.34	-1.35	-3.49	-2.86	-0.74	5.74
				(49.2)	(40.3)	(10.5)	
gag → *ggg*	-0.06	1.32	-1.38	-0.98	-0.08	0.48	-0.80
				(52.7)	(4.3)		(43.0)
gag → *gg⁻g*	-1.34	-0.24	-1.10	-2.85	-2.92	-0.37	5.04
				(46.4)	(47.6)	(6.0)	
gag⁻ → *ggg⁻*	-2.09	0.86	-2.95	-4.20	-1.93	-1.14	4.32
				(57.8)	(26.5)	(15.7)	
gag⁻ → *gg⁻g⁻*	-1.11	0.09	-1.20	-2.87	-2.49	-1.00	5.16
				(45.1)	(39.2)	(15.7)	
ag⁻ 2FE → *gg⁻* 2FE	-2.54	0.57	-3.11	-5.34	-3.03	-0.51	5.77
				(60.1)	(34.1)	(5.8)	
gaa → *gg⁻a*	-1.69	-0.34	-1.35	-3.49	-2.86	-0.74	5.74
gg⁻a → *ag⁻g*	-0.70	1.45	-2.15	-1.84	0.57	3.80	-4.68
gaa → *ag⁻g*[c]	-2.39	1.11	-3.50	-5.33	-2.29	3.06	1.06

gaa → *aag*	0.43	1.13	-0.70	-0.97	-0.16	3.58	-3.15
aag → *ag⁻g*	-2.82	-0.02	-2.80	-4.36	-2.13	-0.52	4.21
gaa → *ag⁻g*[c]	-2.39	1.11	-3.50	-5.33	-2.29	3.06	1.06
gag → *gg⁻a*[c]	*-1.84*	*6.04*	*-7.88*	*-1.01*	*-0.19*	*-3.37*	*-3.31*
				(12.8)	*(2.4)*	*(42.8)*	*(42.0)*

[a] Labeling of various energy terms is the same as in Table 2. Values in italic are in H_2O. Values in parentheses are percentage contribution to all attractive interactions. [b]From ref. 3f. [c]Corresponds to the most stable CC_{anti} → the most stable CC_{gauche} isomerization.

Table S12. Energies of vicinal hyperconjugative interactions between N_3CH_2 and CH_2OH fragments in 2-azidoethanol and their change upon conformational isomerization, estimated on the basis of second-order perturbative approach at the HF/6-311++G(d,p) level.[a] Energies are in kcal/mol.

Conformer	total	$total_{gauche}$	$total_{anti}$	$\sigma_{CH} \rightarrow \sigma^*_{CH}$	$\sigma_{CN3} \rightarrow \sigma^*_{COH}$/ $\sigma_{COH} \rightarrow \sigma^*_{CN3}$	$\sigma_{CH} \rightarrow \sigma^*_{CN3}$/ $\sigma_{CH} \rightarrow \sigma^*_{COH}$	$\sigma_{CN3} \rightarrow \sigma^*_{CH}$/ $\sigma_{COH} \rightarrow \sigma^*_{CH}$
aag	-20.05	-3.88	-16.17	-3.49/-3.25/-2.77/-2.86	-2.18/-1.62		
gaa	-20.13	-4.13	-16.00	-3.32/-2.98/-2.79/-2.97	-1.87/-2.07		
gag	-19.93	-3.78	-16.15	-3.58/-2.96/-2.72/-2.99	-2.13/-1.77		
gag⁻	-19.86	-3.77	-16.09	-3.28/-3.23/-2.83/-2.87	-2.12/-1.76		
ag⁻g	-21.62	-3.85	-17.77	-3.52/-2.92		-4.11/-4.74	-1.26/-1.22
gg⁻a	-21.92	-4.05	-17.87	-3.41/-3.01		-4.50/-4.41	-1.21/-1.33
gg⁻g	-21.97	-3.55	-18.42	-3.47/-2.96		-4.74/-5.00	-1.16/-1.09
ggg⁻	-22.15	-3.79	-18.36	-3.28/-3.08		-4.82/-4.65	-1.28/-1.25
gg⁻g⁻	-22.16	-3.67	-18.49	-3.72/-2.89		-4.47/-5.12	-1.20/-1.09
Isomerization							
aag → *ag⁻g*	-1.57	0.03	-1.60				
gaa → *gg⁻a*	-1.79	0.08	-1.87				
gag → *gg⁻g*	-2.04	0.23	-2.27				
gag⁻ → *ggg⁻*	-2.29	-0.02	-2.27				
gag⁻ → *gg⁻g⁻*	-2.30	0.10	-2.40				

[a] Individual interactions correspond to *anti* vicinal hyperconjugation. $Total_{anti}$ is the sum of six interactions between *anti*-related σ-bonds. $Total_{gauche}$ is the sum of twelve interactions between *gauche*-related σ-bonds. Total is the sum of all vicinal hyperconjugations, that is $total_{anti} + total_{gauche}$.

Table S13. Relative energies (ΔE), enthalpies (ΔH) and free energies (ΔG) for conformers of protonated 2-azidoethanol in the gas-phase and in solvents (CH_2Cl_2, DMSO and H_2O) and energy changes (ΔΔ values) upon conformational isomerizations, obtained at the MP2/6-311++G(d,p) level. All values are in kcal/mol.

Conformer	gas/CH_2Cl_2/DMSO/H_2O		
	ΔE	ΔH	ΔG
aaa, C_1	13.26/5.80/4.80/4.71	14.10/6.53/5.23/5.10	12.62/6.34/4.66/4.45
aag, C_1	**12.73**/**5.48**/4.57/4.48	**13.60**/**5.95**/4.97/4.89	**12.16**/5.31/4.39/4.33
gaa, C_1	- /5.82/4.70/4.59	- /6.37/4.97/4.87	- /5.91/4.30/4.30
gag, C_1	- /5.56/4.53/4.43	- /6.01.4.94/4.82	- /5.46/4.42/4.17
gag$^-$, C_1	- /5.49/**4.43**/**4.33**	- /6.01/**4.83**/**4.71**	- /**5.29**/**4.17**/**4.12**
aga, C_1	1.27/0.73/0.59/0.57	1.40/0.83/0.67/0.64	1.16/0.80/0.70/0.67
agg, C_1	**0.00**/**0.00**/**0.00**/**0.00**	**0.00**/**0.00**/**0.00**/**0.00**	**0.00**/**0.00**/**0.00**/**0.00**
ag$^-$*g*, C_1	- /3.15/2.33/2.25	- /3.54/2.64/2.54	- /3.11/2.28/2.14
gga, C_1	- /1.54/1.31/1.28	- /1.69/1.36/1.31	- /1.61/1.32/1.24
ggg, C_1	- /0.99/0.77/0.75	- /0.95/0.74/0.73	- /0.76/0.58/0.53
ggg$^-$, C_1	- /3.72/2.77/2.68	- /4.12/2.98/2.83	- /3.67/2.27/1.61
gg$^-$*g*, C_1	- /3.63/2.56/2.45	- /3.84/2.71/2.60	- /3.29/2.42/2.39
Isomerization			
aaa → *aga*	-11.99/-5.06/-4.22/-4.14	-12.70/-5.70/-4.56/-4.46	-11.46/-5.54/-3.95/-3.78
aag → *agg*	-12.73/-5.48/-4.57/-4.48	-13.60/-5.95/-4.97/-4.89	-12.16/-5.31/-4.39/-4.33
aag → *ag*$^-$*g*	- /-2.33/-2.24/-2.23	- /-2.41/-2.33/-2.35	- /-2.20/-2.11/-2.19
gaa → *gga*	- /-4.28/-3.40/-3.31	- /-4.67/-3.61/-3.56	- /-4.30/-2.98/-3.06
gag → *ggg*	- /-4.57/-3.76/-3.68	- /-5.06/-4.19/-4.09	- /-4.70/-3.84/-3.64
gag → *gg*$^-$*g*	- /-1.87/-1.97/-1.98	- /-2.16/-2.23/-2.21	- /-2.00/-2.00/-1.78
gag$^-$ → *ggg*$^-$	- /-1.77/-1.66/-1.65	- /-1.89/-1.85/-1.88	- /-1.62/-1.90/-2.51
anti → *gauche*[a]	**-12.73/-5.48/-4.43/-4.33**	**-13.60/-5.95/-4.83/-4.71**	**-12.16/-5.29/-4.17/-4.12**

[a] Energy difference between the most stable CC_{gauche} and the most stable CC_{anti} conformer (bolded numbers for each energy term).

Table S14. Contribution of various energy components to the total binding interactions between $N_3CH_2\cdot$ and $\cdot CH_2OH_2^+$ fragments in the most stable CC_{anti} and CC_{gauche} forms of protonated 2-azidoethanol and energy changes ($\Delta\Delta E$ values) occuring upon conformational isomerization.[a] Data for protonated 2-fluoroethanol (2FEH) are included for comparison.[b] Values are in kcal/mol, obtained at the MP2/6-311++G(d,p) level.

Conformer	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{Pauli}
aag	-112.30	16.31	-128.61	-131.08	-159.24	-39.53	201.24
agg	-124.96	25.57	-150.71	-152.11	-177.53	-46.89	225.82
ag 2FEH	-100.54	12.03	-112.57	-128.21	-145.83	-28.43	198.90
gg 2FEH	-108.77	12.84	-121.61	-140.53	-160.23	-29.27	208.42
gag$^-$	*-106.32*	*15.13*	*-121.45*	*-61.94*	*-233.35*	*-47.54*	*221.38*
ggg$^-$	*-107.97*	*15.72*	*-123.69*	*-65.68*	*-233.82*	*-48.04*	*223.85*
agg	*-110.65*	*20.61*	*-131.26*	*-74.47*	*-226.94*	*-45.84*	*215.99*
Isomerization	ΔE_{iso}	$\Delta\Delta E_{def}$	$\Delta\Delta E_{int}$	$\Delta\Delta E_{elstat}$	$\Delta\Delta E_{oi}$	$\Delta\Delta E_{disp}$	$\Delta\Delta E_{Pauli}$
aag → *agg*[c]	-12.73	9.37	-22.10	-21.03 (45.1)	-18.29 (39.2)	-7.36 (15.7)	24.58
ag 2FEH → *gg* 2FEH	-8.23	0.81	-9.04	-12.32 (66.4)	-5.40 (29.1)	-0.84 (4.5)	9.52
gag$^-$ → *ggg*$^-$	*-1.65*	*0.59*	*-2.24*	*-3.74 (79.4)*	*-0.47 (10.0)*	*-0.50 (10.6)*	*2.47*
ggg$^-$ → *agg*	*-2.68*	*4.89*	*-7.57*	*-8.79 (52.8)*	*6.88*	*2.20*	*-7.86 (47.2)*
gag$^-$ → *agg*[c]	*-4.33*	*5.48*	*-9.81*	*-12.53*	*6.41*	*1.70*	*-5.39*

[a] Labeling of various energy terms is the same as in Table 2. Values in italic are in H_2O. Values in parentheses are percentage contribution to all attractive interactions. [b]From ref. 3f. [c]Corresponds to the most stable CC_{anti} → the most stable CC_{gauche} isomerization.

Table S15. Energies of vicinal hyperconjugative interactions between N_3CH_2 and $CH_2OH_2^+$ fragments in protonated 2-azidoethanol and their changes upon conformational isomerization, estimated on the basis of second-order perturbative approach at the HF/6-311++G(d,p) level.[a] Energies are in kcal/mol.

Conformer	total	$total_{gauche}$	$total_{anti}$	$\sigma_{CH} \rightarrow \sigma^*_{CH}$	$\sigma_{CN3} \rightarrow \sigma^*_{COH2}$/ $\sigma_{COH2} \rightarrow \sigma^*_{CN3}$	$\sigma_{CH} \rightarrow \sigma^*_{CN3}$/ $\sigma_{CH} \rightarrow \sigma^*_{COH2}$	$\sigma_{CN3} \rightarrow \sigma^*_{CH}$/ $\sigma_{COH2} \rightarrow \sigma^*_{CH}$
aaa	-21.52	-4.22	-17.30	-2.68/-2.54/-2.92/-2.88	-5.32/-0.96		
aag	-21.17	-4.56	-16.61	-2.43/-2.55/-2.93/-2.80	-4.82/-1.08		
aga	-18.47	-4.69	-13.78	-2.52/-2.34		-1.81/-4.91	-1.27/-0.93
agg	-18.95	-4.95	-14.00	-2.40/-2.51		-1.85/-4.59	-1.59/-1.06
Isomerization							
aaa → *aga*	3.05	-0.47	3.52				
aag → *agg*	2.22	-0.39	2.61				

[a] Individual interactions correspond to *anti* vicinal hyperconjugation. $Total_{anti}$ is the sum of six interactions between *anti*-related σ-bonds. $Total_{gauche}$ is the sum of twelve interactions between *gauche*-related σ-bonds. Total is the sum of all vicinal hyperconjugations, that is $total_{anti} + total_{gauche}$.

Table S16. Relative energies (ΔE), enthalpies (ΔH) and free energies (ΔG) for nine conformers of *N*-(2-azidoethyl)ethanamide in the gas-phase and in solvents (CH_2Cl_2, DMSO and H_2O) and energy changes (ΔΔ values) upon conformational isomerizations, obtained at the MP2/6-311++G(d,p) level. All values are in kcal/mol.

Conformer	gas/CH_2Cl_2/DMSO/H_2O		
	ΔE	ΔH	ΔG
aag, C_1	3.07/2.38/2.18/2.17	3.00/2.35/2.20/2.22	**1.34**/**0.99**/**1.10**/**1.08**
gag, C_1	**2.68**/**1.90**/**1.75**/**1.74**	**2.70**/**1.99**/**1.85**/**1.88**	1.45/1.36/1.28/1.26
gag$^-$, C_1	3.13/2.21/1.97/1.95	3.13/2.28/2.06/2.08	1.85/1.63/1.52/1.51
agg, C_1	0.91/0.97/1.00/1.02	0.94/0.97/1.00/1.05	**0.00**/0.28/0.30/0.30
ag$^-$*g*, C_1	3.81/2.03/1.54/1.50	3.71/2.00/1.50/1.49	3.09/1.63/1.01/0.93
ggg, C_1	1.59/1.17/1.06/1.06	1.65/1.23/1.11/1.14	0.82/0.73/0.43/0.41
ggg$^-$, C_1	2.21/0.76/0.37/0.34	2.16/0.84/0.46/0.46	2.26/1.14/0.70/0.65
gg$^-$*g*$^-$, C_1	**0.00**/**0.00**/**0.00**/0.01	**0.00**/**0.00**/0.02/0.06	0.11/**0.00**/**0.00**/**0.00**
gg$^-$*g*, C_1	1.70/0.42/0.03/**0.00**	1.58/0.37/**0.00**/**0.00**	1.76/0.94/0.53/0.48
Isomerization			
aag → *agg*	-2.16/-1.41/-1.18/-1.15	-2.06/-1.38/-1.19/-1.17	-1.34/-0.71/-0.80/-0.79
aag → *ag*$^-$*g*	0.74/-0.35/-0.64/-0.67	0.71/-0.35/-0.70/-0.73	0.76/0.64/-0.09/-0.15
gag → *ggg*	-1.09/-0.73/-0.68/-0.68	-1.05/-0.76/-0.74/-0.73	-0.62/-0.62/-0.84/-0.85
gag → *gg*$^-$*g*	-0.98/-1.48/-1.71/-1.74	-1.12/-1.62/-1.85/-1.88	0.31/-0.41/-0.75/-0.79
gag$^-$ → *ggg*$^-$	-0.92/-1.45/-1.60/-1.62	-0.97/-1.44/-1.60/-1.62	0.41/-0.49/-0.82/-0.86
gag$^-$ → *gg*$^-$*g*$^-$	-3.13/-2.21/-1.97/-1.94	-3.13/-2.28/-2.04/-2.02	-1.74/-1.63/-1.52/-1.51
anti → *gauche*[a]	**-2.68**/**-1.90**/**-1.75**/**-1.74**	**-2.70**/**-1.99**/**-1.85**/**-1.88**	**-1.34**/**-0.99**/**-1.10**/**-1.08**

[a] Energy difference between the most stable CC_{gauche} and the most stable CC_{anti} conformer (bolded numbers for each energy term).

Table S17. Contribution of various energy components to the total binding interactions between $N_3CH_2\cdot$ and $\cdot CH_2NHAc$ fragments and energy changes ($\Delta\Delta E$ values) occuring upon conformational isomerization.[a] Values are in kcal/mol, obtained at the MP2/6-311++G(d,p) level.

Conformer	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{oi}	ΔE_{disp}	ΔE_{Pauli}
aag	-102.21	24.67	-126.88	-153.36	-153.61	-48.77	228.86
gag	-102.62	16.68	-119.30	-156.67	-154.80	-49.59	241.76
	-101.96	*15.90*	*-117.87*	*-144.14*	*-167.08*	*-49.20*	*242.55*
gag$^-$	-102.19	16.82	-119.01	-156.04	-154.61	-49.87	241.51
agg	-104.38	25.06	-129.44	-157.26	-154.88	-50.27	232.82
ag$^-$*g*	-101.46	25.92	-127.38	-153.58	-154.14	-50.89	231.23
ggg	-103.74	16.76	-120.50	-159.88	-155.92	-50.27	245.57
ggg$^-$	-103.10	16.05	-119.15	-158.65	-155.57	-50.34	245.41
gg$^-$*g*$^-$	-105.25	17.22	-122.47	-159.25	-156.61	-53.08	246.47
gg$^-$*g*	-103.56	17.65	-121.21	-158.39	-156.64	-53.89	247.71
	-103.73	*17.49*	*-121.20*	*-144.15*	*-171.63*	*-53.42*	*248.00*
Isomerization	ΔE_{iso}	$\Delta\Delta E_{def}$	$\Delta\Delta E_{int}$	$\Delta\Delta E_{elstat}$	$\Delta\Delta E_{oi}$	$\Delta\Delta E_{disp}$	$\Delta\Delta E_{Pauli}$
aag → *agg*	-2.16	0.40	-2.56	-3.90	-1.27	-1.35	3.96
				(59.8)	(19.5)	(20.7)	
aag → *ag*$^-$*g*	0.74	1.24	-0.50	-0.22	-0.53	-2.12	2.37
				(7.7)	(18.5)	(73.8)	
gag → *ggg*	-1.09	0.11	-1.20	-3.21	-1.12	-0.68	3.81
				(64.1)	(22.4)	(13.5)	
gag → *gg*$^-$*g*	-0.98	0.93	-1.91	-1.72	-1.84	-4.30	5.95
				(21.9)	(23.4)	(54.7)	
	-1.74	*1.59*	*-3.33*	*-0.01*	*-4.55*	*-4.22*	*5.45*
				(0.1)	*(51.8)*	*(48.1)*	
gag$^-$ → *ggg*$^-$	-0.92	-0.78	-0.14	-2.61	-0.96	-0.47	3.90
				(64.6)	(23.8)	(11.6)	
gag$^-$ → *gg*$^-$*g*$^-$	-3.13	0.33	-3.46	-3.21	-2.00	-3.21	4.96
				(38.1)	(23.8)	(38.1)	
gag → *gg*$^-$*g*	-0.98	0.93	-1.91	-1.72	-1.84	-4.30	5.95
gg$^-$*g* → *gg*$^-$*g*$^-$	-1.70	-0.44	-1.26	-0.86	0.03	0.81	-1.24
gag → *gg*$^-$*g*$^-$[b]	-2.68	0.49	-3.17	-2.58	-1.81	-3.49	4.71
gag → *gag*$^-$	0.45	0.16	0.29	0.63	0.19	-0.28	-0.25
gag$^-$ → *gg*$^-$*g*$^-$	-3.13	0.33	-3.46	-3.21	-2.00	-3.21	4.96
gag → *gg*$^-$*g*$^-$[b]	-2.68	0.49	-3.17	-2.58	-1.81	-3.49	4.71

[a] Labeling of various energy terms is the same as in Table 2. Values in italic are in H_2O. Values in parentheses are percentage contribution to all attractive interactions. [b]Corresponds to the most stable CC_{anti} → the most stable CC_{gauche} isomerization.

Table S18. Energies of vicinal hyperconjugative interactions between N_3CH_2 and CH_2NHAc fragments in *N*-(2-azidoethyl)ethanamide and their change upon conformational isomerization, estimated on the basis of second-order perturbative approach at the HF/6-311++G(d,p) level.[a] Energies are in kcal/mol.

Conformer	total	$total_{gauche}$	$total_{anti}$	$\sigma_{CH} \rightarrow \sigma^*_{CH}$	$\sigma_{CN3} \rightarrow \sigma^*_{CNHAc}$/ $\sigma_{CNHAc} \rightarrow \sigma^*_{CN3}$	$\sigma_{CH} \rightarrow \sigma^*_{CN3}$/ $\sigma_{CH} \rightarrow \sigma^*_{CNHAc}$	$\sigma_{CN3} \rightarrow \sigma^*_{CH}$/ $\sigma_{CNHAc} \rightarrow \sigma^*_{CH}$
aag	-19.56	-3.69	-15.87	-2.90/-3.28/-3.04/-2.94	-2.21/-1.50		
gag	-19.19	-3.44	-15.75	-2.93/-3.01/-3.01/-3.09	-2.04/-1.67		
gag$^-$	-19.22	-3.52	-15.70	-3.34/-2.62/-2.82/-3.23	-1.95/-1.67		
agg	-20.65	-3.51	-17.14	-3.09/-3.10		-4.01/-4.44	-1.29/-1.24
ggg	-21.03	-3.34	-17.69	-2.83/-3.32		-4.68/-4.63	-1.23/-1.20
ggg$^-$	-20.91	-3.19	-17.72	-3.21/-3.15		-4.49/-4.50	-1.21/-1.16
gg$^-$*g*$^-$	-20.66	-3.27	-17.39	-3.09/-2.99		-4.50/-4.56	-1.22/-1.03
gg$^-$*g*	-21.13	-3.45	-17.68	-3.54/-2.88		-4.44/-4.56	-1.21/-1.05
Isomerization							
aag $\rightarrow$ *agg*	-1.09	0.18	-1.27				
gag $\rightarrow$ *ggg*	-1.84	0.10	-1.94				
gag $\rightarrow$ *gg*$^-$*g*	-1.94	-0.01	-1.93				
gag$^-$ $\rightarrow$ *ggg*$^-$	-1.69	0.33	-2.02				
gag$^-$ $\rightarrow$ *gg*$^-$*g*$^-$	-1.44	0.25	-1.69				

[a] Individual interactions correspond to *anti* vicinal hyperconjugation. $Total_{anti}$ is the sum of six interactions between *anti*-related σ-bonds. $Total_{gauche}$ is the sum of twelve interactions between *gauche*-related σ-bonds. Total is the sum of all vicinal hyperconjugations, that is $total_{anti} + total_{gauche}$.

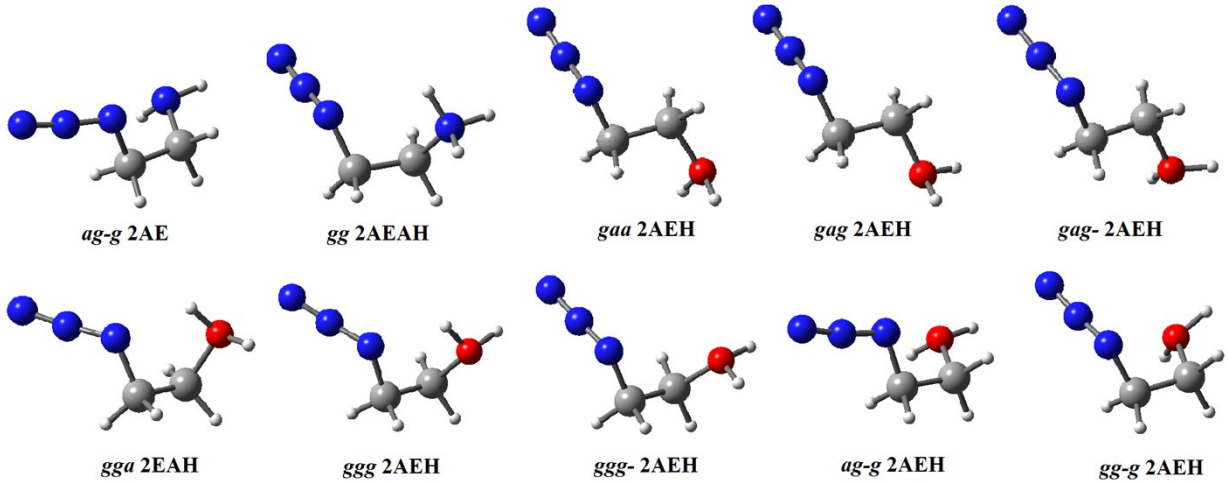

Figure S1. Optimized structures of isomers which are viable only in solvents (2AE: 2-azidoethanamine, in DMSO; 2AEAH: 2-azidoethylammonium ion, in CH_2Cl_2; 2AEH: protonated 2-azidoethanol, in CH_2Cl_2).

Absolute energies (a.u.) and x,y,z coordinates (Å) of optimized structures

Gas-phase

1,2-Diazidoethane

aaa, E = -406.1931001 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.392131	0.648500	0.089922
2	1	0	-1.053476	0.678566	0.963125
3	1	0	-0.999367	0.718517	-0.819391
4	6	0	0.392131	-0.648500	0.089922
5	1	0	0.999367	-0.718517	-0.819391
6	1	0	1.053476	-0.678566	0.963125
7	7	0	0.601382	1.737049	0.150272
8	7	0	0.146174	2.872289	-0.044045
9	7	0	-0.146174	3.977155	-0.203837
10	7	0	-0.601382	-1.737049	0.150272
11	7	0	-0.146174	-2.872289	-0.044045
12	7	0	0.146174	-3.977155	-0.203837

aag, E = -406.1931737 a.u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.396383	0.023885	0.234218
2	1	0	-0.517906	0.065169	1.322712
3	1	0	-0.100062	-0.993522	-0.051697
4	6	0	0.666280	1.023460	-0.196519
5	1	0	0.767906	1.015696	-1.287784
6	1	0	0.387115	2.027237	0.122066
7	7	0	-1.643287	0.405332	-0.456815
8	7	0	-2.657208	-0.188532	-0.063684
9	7	0	-3.672073	-0.667537	0.205146
10	7	0	1.953499	0.732410	0.459428
11	7	0	2.530046	-0.286262	0.048695
12	7	0	3.180959	-1.195218	-0.240126

gag, E = -406.1933327 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.745854	0.164269	-0.696479
2	1	0	-1.000291	0.726072	-1.595021
3	1	0	-1.006495	0.770030	0.181082
4	6	0	0.745854	-0.164269	-0.696479
5	1	0	1.006495	-0.770030	0.181082
6	1	0	1.000291	-0.726072	-1.595021
7	7	0	-1.559430	-1.064415	-0.738490

8	7	0	-1.559430	-1.722749	0.313369
9	7	0	-1.661278	-2.425294	1.224094
10	7	0	1.559430	1.064415	-0.738490
11	7	0	1.559430	1.722749	0.313369
12	7	0	1.661278	2.425294	1.224094

***gag*⁻**, E = -406.1932421 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.364319	-0.615404	0.267235
2	1	0	0.364673	-0.614970	1.358492
3	1	0	1.402901	-0.614856	-0.083019
4	6	0	-0.364319	0.615404	-0.267235
5	1	0	-0.364673	0.614970	-1.358492
6	1	0	-1.402901	0.614856	0.083019
7	7	0	-0.330916	-1.854737	-0.125585
8	7	0	-0.246061	-2.137365	-1.330644
9	7	0	-0.242874	-2.527594	-2.417214
10	7	0	0.330916	1.854737	0.125585
11	7	0	0.246061	2.137365	1.330644
12	7	0	0.242874	2.527594	2.417214

aga, E = -406.1936685 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.292630	-0.696986	1.117079
2	1	0	-0.039286	-1.202426	2.056564
3	1	0	-1.382869	-0.632062	1.025339
4	6	0	0.292630	0.696986	1.117079
5	1	0	0.039286	1.202426	2.056564
6	1	0	1.382869	0.632062	1.025339
7	7	0	-0.292630	1.427276	-0.022068
8	7	0	0.383949	2.374732	-0.443643
9	7	0	0.292630	-1.427276	-0.022068
10	7	0	-0.383949	-2.374732	-0.443643
11	7	0	0.914242	3.275492	-0.932057
12	7	0	-0.914242	-3.275492	-0.932057

agg, E = -406.1932735 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.906857	1.389773	0.080560
2	1	0	-1.550880	1.767528	0.884861
3	1	0	-0.681371	2.207731	-0.603671
4	6	0	0.378055	0.850487	0.681890
5	1	0	0.830843	1.622951	1.316330
6	1	0	0.165672	-0.027350	1.306767
7	7	0	1.284137	0.500126	-0.424592
8	7	0	2.182869	-0.301430	-0.134906

9	7	0	-1.625843	0.389286	-0.727665
10	7	0	-1.956749	-0.633710	-0.112494
11	7	0	3.064319	-1.033664	-0.000669
12	7	0	-2.318940	-1.636668	0.331898

agg⁻, E = -406.1958291 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.033889	1.392405	0.231114
2	1	0	1.419543	2.364914	-0.078897
3	1	0	1.182225	1.281201	1.311880
4	6	0	-0.446126	1.310399	-0.091526
5	1	0	-0.974266	2.153448	0.372226
6	1	0	-0.586919	1.344468	-1.177997
7	7	0	-0.937327	0.032527	0.459318
8	7	0	-2.045148	-0.332759	0.043763
9	7	0	1.820014	0.398373	-0.514066
10	7	0	1.752665	-0.768283	-0.092924
11	7	0	-3.064509	-0.780577	-0.259095
12	7	0	1.821854	-1.886546	0.182326

ggg, =-406.1937411 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.716793	-0.260402	1.053264
2	1	0	-0.873040	-0.877350	1.948005
3	1	0	-1.429096	0.566374	1.081719
4	6	0	0.716793	0.260402	1.053264
5	1	0	0.873040	0.877350	1.948005
6	1	0	1.429096	-0.566374	1.081719
7	7	0	1.052576	1.012300	-0.167066
8	7	0	0.306309	1.971417	-0.410543
9	7	0	-1.052576	-1.012300	-0.167066
10	7	0	-0.306309	-1.971417	-0.410543
11	7	0	-0.306309	2.886692	-0.758006
12	7	0	0.306309	-2.886692	-0.758006

g⁻gg⁻, E = -406.1960389 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.149653	1.324984	0.051007
2	1	0	1.736177	2.101338	-0.444953
3	1	0	1.442416	1.276711	1.106030
4	6	0	-0.332390	1.666461	-0.058035
5	1	0	-0.513318	2.638547	0.406913
6	1	0	-0.625047	1.715673	-1.112584
7	7	0	-1.161132	0.695829	0.677947
8	7	0	-1.586385	-0.258925	0.008610
9	7	0	1.475156	0.069764	-0.644266

10	7	0	1.236831	-0.969994	-0.007895
11	7	0	-2.059291	-1.189256	-0.484297
12	7	0	1.102849	-2.016124	0.462296

***ggg*⁻**, E = -406.1956305 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.455534	1.490525	-0.389206
2	1	0	-1.240285	2.143256	0.015518
3	1	0	-0.011787	1.965160	-1.264222
4	6	0	0.615332	1.255164	0.669228
5	1	0	1.016096	2.215135	1.000432
6	1	0	0.186403	0.744279	1.542224
7	7	0	1.761789	0.503439	0.139399
8	7	0	1.563070	-0.708435	-0.045316
9	7	0	-1.031338	0.224660	-0.881508
10	7	0	-1.673019	-0.418487	-0.037436
11	7	0	1.545479	-1.846241	-0.239186
12	7	0	-2.295868	-1.118073	0.639179

2-Azidoethanamine

aaa, E = -298.1418011 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.499081	0.736702	0.000000
2	1	0	-1.945313	0.266175	0.880166
3	1	0	-1.945313	0.266175	-0.880166
4	6	0	0.000000	0.457283	0.000000
5	1	0	0.464681	0.899471	-0.891198
6	1	0	0.464681	0.899471	0.891198
7	7	0	0.189361	-1.009780	0.000000
8	7	0	1.368633	-1.384237	0.000000
9	7	0	2.420225	-1.862078	0.000000
10	7	0	-1.847969	2.150787	0.000000
11	1	0	-1.477998	2.620980	0.818923
12	1	0	-1.477998	2.620980	-0.818923

aag, E = -298.1422118 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.578301	0.496007	-0.044005
2	1	0	1.577205	1.198243	0.800750
3	1	0	1.558983	1.084828	-0.964353
4	6	0	0.315297	-0.344189	0.024321
5	1	0	0.233009	-0.959696	-0.877977
6	1	0	0.351551	-1.007449	0.898417
7	7	0	-0.833263	0.579780	0.142918

8	7	0	-1.944619	0.053391	0.008670
9	7	0	-3.035777	-0.311357	-0.093802
10	7	0	2.733941	-0.397746	-0.088510
11	1	0	3.570913	0.111684	-0.347643
12	1	0	2.904779	-0.806991	0.823980

gaa, E = -298.1422683 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.194424	-0.348147	-0.376710
2	1	0	1.204244	-0.181801	-1.457428
3	1	0	0.676766	-1.297294	-0.202367
4	6	0	0.405442	0.784587	0.284666
5	1	0	0.364038	0.634386	1.371935
6	1	0	0.885111	1.745535	0.090458
7	7	0	-0.959651	0.909794	-0.267824
8	7	0	-1.714670	-0.038488	-0.012211
9	7	0	-2.526320	-0.843743	0.156285
10	7	0	2.567727	-0.486356	0.088501
11	1	0	3.099839	0.358541	-0.089685
12	1	0	2.601206	-0.666454	1.086089

gag, E = -298.1424994 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.183509	-0.368995	0.331280
2	1	0	-1.143382	-0.282628	1.426018
3	1	0	-0.696822	-1.310208	0.056244
4	6	0	-0.400772	0.789763	-0.275126
5	1	0	-0.357972	0.680079	-1.364363
6	1	0	-0.885521	1.739642	-0.043109
7	7	0	0.957468	0.897839	0.297651
8	7	0	1.715907	-0.040325	0.017847
9	7	0	2.528778	-0.840586	-0.167200
10	7	0	-2.532877	-0.373863	-0.229932
11	1	0	-3.013707	-1.236966	-0.002585
12	1	0	-3.081842	0.384017	0.162301

gag^{-}, E = -298.1424243 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.201519	-0.309609	-0.390991
2	1	0	1.265543	-0.096310	-1.461068
3	1	0	0.662452	-1.262102	-0.275264
4	6	0	0.398706	0.802797	0.272790
5	1	0	0.357962	0.648616	1.359325
6	1	0	0.870173	1.765538	0.080143
7	7	0	-0.968828	0.899500	-0.277991
8	7	0	-1.710631	-0.055548	-0.011796

9	7	0	-2.511875	-0.869179	0.166019
10	7	0	2.552145	-0.319186	0.166029
11	1	0	2.549764	-0.705315	1.104265
12	1	0	3.167082	-0.898669	-0.394029

aga, E = -298.1440541 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.745098	0.495856	-0.198174
2	1	0	-1.801322	0.638825	-1.281333
3	1	0	-2.410465	1.232869	0.262800
4	6	0	-0.320970	0.790767	0.255958
5	1	0	-0.037656	1.818531	-0.005748
6	1	0	-0.237240	0.664264	1.343590
7	7	0	0.568963	-0.171263	-0.432180
8	7	0	1.751968	-0.143386	-0.071187
9	7	0	2.878454	-0.212968	0.174251
10	7	0	-2.235780	-0.837493	0.114295
11	1	0	-1.610550	-1.532875	-0.280624
12	1	0	-2.251588	-0.985581	1.118355

agg, E = -298.1448704 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.746055	0.487262	0.171759
2	1	0	1.825320	0.645749	1.257260
3	1	0	2.419265	1.194462	-0.322387
4	6	0	0.329801	0.810085	-0.256076
5	1	0	0.079976	1.849944	-0.014680
6	1	0	0.229369	0.644492	-1.334723
7	7	0	-0.570449	-0.105134	0.485687
8	7	0	-1.738922	-0.135729	0.080374
9	7	0	-2.853166	-0.252784	-0.199486
10	7	0	2.086439	-0.863388	-0.263724
11	1	0	3.041435	-1.090340	-0.007797
12	1	0	1.482193	-1.529147	0.208267

gga, E = -298.1437475 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.316782	-0.042311	0.676249
2	1	0	0.707286	-0.691260	1.315405
3	1	0	2.077648	0.410437	1.321052
4	6	0	0.435868	1.073254	0.114974
5	1	0	0.013513	1.680797	0.926397
6	1	0	1.014491	1.723974	-0.543289
7	7	0	-0.650764	0.535802	-0.736703
8	7	0	-1.526808	-0.087607	-0.121040
9	7	0	-2.412751	-0.679856	0.326056

10	7	0	1.982548	-0.873328	-0.316288
11	1	0	1.300072	-1.258782	-0.961382
12	1	0	2.625514	-0.315899	-0.869690

ggg, E = -298.1443563 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.310068	-0.031264	0.670083
2	1	0	0.688987	-0.687503	1.301140
3	1	0	2.069537	0.420035	1.316871
4	6	0	0.436238	1.081087	0.115673
5	1	0	0.015248	1.686297	0.927361
6	1	0	1.022500	1.718555	-0.545911
7	7	0	-0.655799	0.541349	-0.731583
8	7	0	-1.518313	-0.097432	-0.113026
9	7	0	-2.391740	-0.705804	0.337542
10	7	0	1.980554	-0.716402	-0.429387
11	1	0	2.531487	-1.495718	-0.085905
12	1	0	1.291486	-1.092581	-1.072913

***ggg*$^-$**, E = -298.1417039 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.288352	-0.052366	0.620635
2	1	0	0.695693	-0.570123	1.382517
3	1	0	2.197425	0.321454	1.117094
4	6	0	0.517976	1.164685	0.126331
5	1	0	0.292491	1.821384	0.976045
6	1	0	1.115590	1.733972	-0.589104
7	7	0	-0.725746	0.833384	-0.596109
8	7	0	-1.412767	-0.056343	-0.081346
9	7	0	-2.141541	-0.874490	0.284325
10	7	0	1.528245	-0.989400	-0.470182
11	1	0	2.103109	-0.561957	-1.189128
12	1	0	2.020379	-1.810700	-0.136036

g*$^-$*ga, E = -298.1432959 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.668685	-0.108686	-0.131111
2	1	0	1.882664	-0.338759	-1.178489
3	1	0	2.579260	-0.318098	0.442047
4	6	0	0.578649	-1.060192	0.363969
5	1	0	0.902277	-2.096758	0.245986
6	1	0	0.367618	-0.880283	1.426541
7	7	0	-0.665143	-0.939199	-0.425770
8	7	0	-1.436707	-0.037460	-0.073939
9	7	0	-2.263104	0.734844	0.164831
10	7	0	1.372570	1.311586	-0.033442

11	1	0	0.626317	1.581725	-0.663130
12	1	0	1.104545	1.577043	0.908133

g⁻gg, E = -298.1440396 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.681067	-0.127767	-0.094023
2	1	0	1.974632	-0.384178	-1.121217
3	1	0	2.545670	-0.299417	0.555485
4	6	0	0.570136	-1.067977	0.348179
5	1	0	0.868907	-2.108126	0.202806
6	1	0	0.341538	-0.901221	1.406587
7	7	0	-0.643958	-0.880973	-0.475641
8	7	0	-1.443075	-0.026087	-0.068145
9	7	0	-2.288786	0.713029	0.200314
10	7	0	1.242076	1.257128	0.067070
11	1	0	2.035665	1.887439	0.083227
12	1	0	0.662574	1.538293	-0.717007

g⁻gg⁻, E = -298.1441097 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.607005	-0.099465	-0.228892
2	1	0	1.631050	-0.240582	-1.312631
3	1	0	2.603919	-0.347945	0.166940
4	6	0	0.600827	-1.080849	0.355571
5	1	0	0.948086	-2.105591	0.212412
6	1	0	0.486043	-0.906508	1.434522
7	7	0	-0.705577	-1.014881	-0.317007
8	7	0	-1.407075	-0.023906	-0.064522
9	7	0	-2.196765	0.804142	0.087294
10	7	0	1.174327	1.267370	0.047448
11	1	0	1.371776	1.520258	1.010257
12	1	0	1.657772	1.933169	-0.544067

2-Azidoethylammonium ion

aa, E = -298.4896945 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.461809	0.531699	-0.052287
2	1	0	1.499362	1.225841	0.787701
3	1	0	1.474295	1.088431	-0.989291
4	6	0	0.237243	-0.365491	0.041136
5	1	0	0.187007	-1.033839	-0.830079
6	1	0	0.280279	-0.976441	0.954638
7	7	0	-0.875805	0.579286	0.074558
8	7	0	-2.002694	0.045682	0.002219

9	7	0	-3.095822	-0.303905	-0.052915
10	7	0	2.724460	-0.293663	-0.005821
11	1	0	2.793411	-0.823332	0.868639
12	1	0	2.761567	-0.966994	-0.777329
13	1	0	3.558788	0.297283	-0.073664

ag, E = -298.4877987 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.184091	-0.291489	-0.428125
2	1	0	1.283001	0.015045	-1.469905
3	1	0	0.800775	-1.312039	-0.381331
4	6	0	0.296646	0.689036	0.337482
5	1	0	0.175429	0.374861	1.382912
6	1	0	0.741210	1.688312	0.325161
7	7	0	-0.979494	0.804424	-0.361990
8	7	0	-1.830779	-0.046814	-0.022849
9	7	0	-2.719293	-0.744139	0.193375
10	7	0	2.578694	-0.322911	0.159263
11	1	0	3.014543	0.604102	0.125301
12	1	0	2.567668	-0.621490	1.139461
13	1	0	3.189057	-0.967988	-0.352334

ga, E = -298.5033931 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.662546	0.601286	-0.266265
2	1	0	-1.684610	0.637392	-1.355631
3	1	0	-2.410269	1.277646	0.148445
4	6	0	-0.263232	0.880439	0.257179
5	1	0	0.096499	1.812030	-0.191970
6	1	0	-0.263870	0.992453	1.349087
7	7	0	0.520843	-0.292158	-0.160424
8	7	0	1.758967	-0.173709	-0.045783
9	7	0	2.904896	-0.177314	0.013338
10	7	0	-2.028278	-0.808145	0.117584
11	1	0	-1.230607	-1.411712	-0.138571
12	1	0	-2.174034	-0.902895	1.126721
13	1	0	-2.873438	-1.135987	-0.356561

2-Azidoethanol

aaa, E = -317.9936287 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.583141	0.475521	-0.084728
2	1	0	-1.534298	0.984153	-1.054246
3	1	0	-1.637358	1.231104	0.707517

4	6	0	-0.332424	-0.355839	0.112297
5	1	0	-0.397712	-0.899388	1.060953
6	1	0	-0.234440	-1.077152	-0.706466
7	7	0	0.807909	0.582533	0.131462
8	7	0	1.921124	0.060009	-0.002456
9	7	0	3.012890	-0.299114	-0.111987
10	1	0	-3.484966	0.080731	-0.105723
11	8	0	-2.676413	-0.430192	-0.023323

aag, E = -317.9931043 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.591839	0.489064	-0.066091
2	1	0	-1.558875	1.046658	-1.002686
3	1	0	-1.642427	1.206877	0.760766
4	6	0	-0.333193	-0.352850	0.071738
5	1	0	-0.381802	-0.960313	0.985220
6	1	0	-0.244027	-1.022601	-0.790800
7	7	0	0.810086	0.578567	0.145862
8	7	0	1.922547	0.054860	0.005299
9	7	0	3.013663	-0.305314	-0.106790
10	1	0	-2.858274	-0.746538	0.730287
11	8	0	-2.748559	-0.329770	-0.128409

gaa, E = -317.9937883 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.217348	-0.344669	0.363449
2	1	0	-1.282010	-0.169871	1.443584
3	1	0	-0.706471	-1.301653	0.192777
4	6	0	-0.419856	0.782062	-0.271693
5	1	0	-0.362122	0.634856	-1.355968
6	1	0	-0.902710	1.738060	-0.072735
7	7	0	0.928822	0.876774	0.320873
8	7	0	1.701003	-0.043728	0.017572
9	7	0	2.528421	-0.823434	-0.187331
10	1	0	-3.053011	-0.963340	0.206036
11	8	0	-2.497271	-0.328712	-0.252754

gag, E = -317.9932137 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.219109	-0.334477	0.389783
2	1	0	-1.285520	-0.128940	1.458999
3	1	0	-0.706009	-1.296206	0.256999
4	6	0	-0.423865	0.776883	-0.287973
5	1	0	-0.369048	0.604363	-1.371501
6	1	0	-0.909747	1.736830	-0.115863
7	7	0	0.931860	0.896495	0.281896

8	7	0	1.698001	-0.040409	0.014394
9	7	0	2.521602	-0.830580	-0.164625
10	1	0	-2.518406	-0.655385	-1.015308
11	8	0	-2.551707	-0.386705	-0.093231

***gag*⁻**, E = -317.993299 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.211726	-0.369907	0.355741
2	1	0	-1.246155	-0.220396	1.441236
3	1	0	-0.715722	-1.323131	0.158482
4	6	0	-0.424351	0.767676	-0.286831
5	1	0	-0.370011	0.616126	-1.370894
6	1	0	-0.912025	1.725529	-0.095980
7	7	0	0.923362	0.891050	0.301911
8	7	0	1.703020	-0.030304	0.018879
9	7	0	2.536649	-0.807292	-0.169540
10	1	0	-3.004953	0.300962	0.046828
11	8	0	-2.509487	-0.482485	-0.206486

agg, E = -317.9921166 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.756580	0.442143	-0.140913
2	1	0	-1.839055	0.643634	-1.210263
3	1	0	-2.443514	1.112470	0.393312
4	6	0	-0.343570	0.748212	0.317465
5	1	0	-0.165874	1.829629	0.251924
6	1	0	-0.213712	0.441374	1.364717
7	7	0	0.601122	0.025823	-0.552682
8	7	0	1.742228	-0.110362	-0.095528
9	7	0	2.838174	-0.305520	0.211414
10	1	0	-2.048051	-1.120474	0.965227
11	8	0	-2.119945	-0.914793	0.029169

***agg*⁻**, E = -317.9975925 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.769865	0.432869	0.162376
2	1	0	1.877186	0.565816	1.246226
3	1	0	2.481718	1.089393	-0.342360
4	6	0	0.361145	0.812312	-0.247646
5	1	0	0.151734	1.857083	0.011957
6	1	0	0.241168	0.667594	-1.327172
7	7	0	-0.549747	-0.090944	0.493424
8	7	0	-1.716056	-0.120341	0.079270
9	7	0	-2.829291	-0.229829	-0.204898
10	1	0	1.421680	-1.454368	0.175797
11	8	0	2.088263	-0.888601	-0.228425

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gga, =-317.9931951 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.287412	-0.128280	0.624199
2	1	0	0.642741	-0.831485	1.168823
3	1	0	2.071821	0.217366	1.311107
4	6	0	0.474800	1.074197	0.187887
5	1	0	0.152677	1.636642	1.073748
6	1	0	1.086664	1.723372	-0.438509
7	7	0	-0.694028	0.718517	-0.640479
8	7	0	-1.488658	-0.066018	-0.108883
9	7	0	-2.304063	-0.796174	0.262457
10	1	0	2.145573	-1.605854	-0.298796
11	8	0	1.841812	-0.726227	-0.535070

ggg, E = -317.9933057 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.306798	-0.119325	0.623375
2	1	0	0.701612	-0.729714	1.298868
3	1	0	2.183525	0.233778	1.183791
4	6	0	0.514893	1.097828	0.167006
5	1	0	0.231645	1.693078	1.045643
6	1	0	1.121324	1.728696	-0.486683
7	7	0	-0.676229	0.757907	-0.632311
8	7	0	-1.451894	-0.046205	-0.098718
9	7	0	-2.256076	-0.785119	0.277083
10	1	0	2.141145	-0.454159	-1.094366
11	8	0	1.672500	-0.978598	-0.438990

ggg^{-}, E = -317.9966316 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.343019	-0.068464	0.659246
2	1	0	0.740559	-0.734737	1.293251
3	1	0	2.136631	0.360840	1.275624
4	6	0	0.466104	1.045594	0.113269
5	1	0	0.044279	1.646081	0.928634
6	1	0	1.048720	1.688919	-0.546040
7	7	0	-0.615200	0.492960	-0.738676
8	7	0	-1.518883	-0.081719	-0.112812
9	7	0	-2.430652	-0.623832	0.344383
10	1	0	1.290027	-1.043147	-1.000717
11	8	0	1.979773	-0.786574	-0.379513

g^{-}***ga***, E = -317.9964716 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.603310	-0.012971	-0.214404
2	1	0	1.660519	-0.128211	-1.302867
3	1	0	2.600749	-0.166688	0.218607
4	6	0	0.654399	-1.052728	0.343741
5	1	0	1.055431	-2.052416	0.170072
6	1	0	0.540027	-0.900639	1.423917
7	7	0	-0.653950	-1.028735	-0.329130
8	7	0	-1.382357	-0.060239	-0.062333
9	7	0	-2.184877	0.753885	0.094136
10	1	0	1.545349	1.931109	-0.352833
11	8	0	1.074994	1.257083	0.143546

g⁻gg, E = -317.9950677 a.u

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.595566	-0.011512	-0.236458
2	1	0	1.639990	-0.144662	-1.318606
3	1	0	2.602397	-0.156220	0.177793
4	6	0	0.653947	-1.047360	0.356878
5	1	0	1.056517	-2.050164	0.200122
6	1	0	0.544426	-0.887453	1.438994
7	7	0	-0.662356	-1.042904	-0.298265
8	7	0	-1.383154	-0.062059	-0.059654
9	7	0	-2.180507	0.760231	0.083570
10	1	0	1.231552	1.515392	0.907390
11	8	0	1.126270	1.311183	-0.025972

g⁻gg⁻, E = -317.9953487 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.658495	-0.039146	-0.126116
2	1	0	1.883447	-0.219364	-1.183061
3	1	0	2.576002	-0.177599	0.452882
4	6	0	0.620170	-1.043535	0.348649
5	1	0	0.986853	-2.060629	0.194518
6	1	0	0.418641	-0.894523	1.415552
7	7	0	-0.627624	-0.940761	-0.433976
8	7	0	-1.414838	-0.055787	-0.066763
9	7	0	-2.256375	0.697355	0.174863
10	1	0	0.710548	1.568853	-0.668226
11	8	0	1.230547	1.296712	0.091784

Protonated 2-azidoethanol

aaa, E = -318.2854237 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.423838	0.526903	-0.142003
2	1	0	1.521015	1.317156	0.599738
3	1	0	1.436714	0.934539	-1.150041
4	6	0	0.253341	-0.396225	0.133148
5	1	0	0.142561	-1.131046	-0.674622
6	1	0	0.388995	-0.923784	1.087349
7	7	0	-0.856293	0.552480	0.191445
8	7	0	-1.982417	0.043305	0.005029
9	7	0	-3.073067	-0.283900	-0.141905
10	1	0	2.970879	-0.529699	0.849410
11	1	0	2.856584	-0.940345	-0.682639
12	8	0	2.750328	-0.211761	-0.044756

aag, E = -318.2862642 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.419317	0.529149	-0.101208
2	1	0	1.508755	1.252642	0.707841
3	1	0	1.433467	1.002307	-1.080193
4	6	0	0.250283	-0.414779	0.085707
5	1	0	0.135378	-1.055745	-0.795060
6	1	0	0.394743	-1.043330	0.975904
7	7	0	-0.855421	0.524594	0.266602
8	7	0	-1.982364	0.048631	0.011161
9	7	0	-3.073177	-0.253250	-0.181434
10	1	0	3.490426	0.174012	-0.371408
11	1	0	2.864401	-0.758832	0.752431
12	8	0	2.691495	-0.312137	-0.096351

aga, E = -318.3045322 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.766490	0.518932	-0.154884
2	1	0	-1.995110	0.635982	-1.211384
3	1	0	-2.544458	0.950194	0.471400
4	6	0	-0.348896	0.967287	0.196600
5	1	0	-0.115800	1.893998	-0.334947
6	1	0	-0.227329	1.116073	1.275005
7	7	0	0.454884	-0.177173	-0.279497
8	7	0	1.685024	-0.134181	-0.047979
9	7	0	2.820731	-0.173520	0.090156
10	1	0	-0.776890	-1.180551	-0.066402
11	1	0	-2.103070	-1.240825	0.920403
12	8	0	-1.783687	-0.962259	0.044609

agg, E = -318.3065567 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.776665	0.504632	0.125923
2	1	0	2.030318	0.575684	1.183114
3	1	0	2.529471	0.958480	-0.513465
4	6	0	0.356125	0.977481	-0.163702
5	1	0	0.158984	1.909900	0.371160
6	1	0	0.203462	1.118477	-1.238349
7	7	0	-0.453288	-0.151694	0.349103
8	7	0	-1.673780	-0.130041	0.059073
9	7	0	-2.802178	-0.186789	-0.124278
10	1	0	2.350774	-1.499908	0.249493
11	1	0	0.720590	-1.144436	0.020174
12	8	0	1.714298	-0.941401	-0.229092

N-(2-Azidoethyl)ethanamide

aag, E = -450.5017572 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.140306	1.008770	-0.485202
2	1	0	-0.121590	2.069036	-0.508826
3	1	0	0.159020	0.628685	-1.509413
4	6	0	-0.902211	0.238215	0.313639
5	1	0	-0.669848	-0.830709	0.277342
6	1	0	-0.900436	0.577021	1.356989
7	7	0	-2.212325	0.517999	-0.310881
8	7	0	-3.140974	-0.202911	0.076123
9	7	0	-4.089321	-0.800226	0.353513
10	7	0	1.460870	0.868600	0.095166
11	1	0	1.850498	1.622115	0.638176
12	6	0	2.183407	-0.281792	-0.074035
13	6	0	3.561142	-0.290116	0.551668
14	1	0	3.764021	0.592293	1.162120
15	1	0	3.658822	-1.186818	1.165773
16	1	0	4.302149	-0.349670	-0.248544
17	8	0	1.741719	-1.232081	-0.708436

gag, E = -450.5023757 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.097848	-0.763771	-0.659378
2	1	0	0.374848	-1.615305	-1.285193
3	1	0	0.345023	0.158120	-1.194649
4	6	0	0.874035	-0.813017	0.657019
5	1	0	0.571788	0.024334	1.294118
6	1	0	0.674541	-1.749896	1.178785
7	7	0	2.330039	-0.794856	0.415925
8	7	0	2.777854	0.290865	0.016428
9	7	0	3.335365	1.234627	-0.347167
10	7	0	-1.333437	-0.792200	-0.434644

11	1	0	-1.844353	-1.650579	-0.564253
12	6	0	-1.994451	0.331354	-0.015054
13	6	0	-3.488329	0.184594	0.172501
14	1	0	-3.842505	-0.839154	0.035064
15	1	0	-3.748043	0.526693	1.175733
16	1	0	-3.991215	0.837135	-0.544483
17	8	0	-1.405431	1.388080	0.177569

***gag*⁻**, E = -450.5016516 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.168400	-0.359972	-0.512458
2	1	0	-0.078189	0.265187	-1.404149
3	1	0	-0.763451	-1.242890	-0.763803
4	6	0	-0.851390	0.446977	0.592306
5	1	0	-0.919973	-0.149891	1.510596
6	1	0	-0.276196	1.349148	0.794124
7	7	0	-2.190947	0.904543	0.172162
8	7	0	-3.028402	0.002720	0.031107
9	7	0	-3.907160	-0.730764	-0.129659
10	7	0	1.151594	-0.802553	-0.110422
11	1	0	1.283998	-1.744955	0.220087
12	6	0	2.207043	0.070687	-0.092743
13	6	0	3.532469	-0.511063	0.347916
14	1	0	3.459763	-1.547256	0.684695
15	1	0	4.228518	-0.455631	-0.491813
16	1	0	3.931780	0.105728	1.154850
17	8	0	2.079977	1.240395	-0.432128

agg, E = -450.5051956 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.246738	1.478844	-0.430530
2	1	0	0.080698	1.990471	-1.338754
3	1	0	-0.808342	2.180806	0.189522
4	6	0	0.958689	0.985444	0.353117
5	1	0	1.615494	1.827040	0.605331
6	1	0	0.622799	0.497633	1.274360
7	7	0	1.669543	0.019907	-0.516085
8	7	0	2.658949	-0.517797	-0.001603
9	7	0	3.596120	-1.086593	0.361102
10	7	0	-1.133166	0.396631	-0.805701
11	1	0	-0.869836	-0.161695	-1.604094
12	6	0	-1.934074	-0.187192	0.142748
13	6	0	-2.636717	-1.454713	-0.290814
14	1	0	-2.593439	-1.618168	-1.369435
15	1	0	-2.170007	-2.301585	0.219014
16	1	0	-3.678098	-1.402320	0.029477
17	8	0	-2.073294	0.296060	1.260434

***agg*⁻**, E = -450.5005642 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.257582	1.609736	0.074635
2	1	0	0.425893	1.541018	1.150717
3	1	0	0.415747	2.646829	-0.239882
4	6	0	-1.172003	1.207394	-0.254245
5	1	0	-1.870998	1.853593	0.291786
6	1	0	-1.363115	1.317936	-1.330718
7	7	0	-1.342854	-0.203569	0.141757
8	7	0	-2.499199	-0.633490	0.045286
9	7	0	-3.529265	-1.154127	-0.000197
10	7	0	1.224254	0.737651	-0.555168
11	1	0	1.152666	0.600316	-1.553063
12	6	0	1.865828	-0.247851	0.164852
13	6	0	2.573053	-1.282702	-0.683298
14	1	0	2.864177	-0.895710	-1.662638
15	1	0	3.456071	-1.633482	-0.149535
16	1	0	1.896710	-2.130574	-0.825602
17	8	0	1.863193	-0.280581	1.385689

ggg, E = -450.504104 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.139059	0.778928	0.876358
2	1	0	-0.842819	0.502037	1.667355
3	1	0	0.402026	1.673475	1.194684
4	6	0	-0.884672	1.090011	-0.417766
5	1	0	-1.561278	1.941335	-0.272137
6	1	0	-0.173163	1.333652	-1.205552
7	7	0	-1.637758	-0.088301	-0.905404
8	7	0	-2.617737	-0.399821	-0.214793
9	7	0	-3.556352	-0.794688	0.332654
10	7	0	0.819125	-0.296030	0.718613
11	1	0	0.479643	-1.245219	0.758046
12	6	0	1.995314	-0.064320	0.050331
13	6	0	2.822293	-1.293016	-0.255944
14	1	0	2.505284	-2.171270	0.310046
15	1	0	2.741100	-1.507978	-1.324717
16	1	0	3.867376	-1.073054	-0.034843
17	8	0	2.345954	1.066161	-0.266031

***ggg*$^{-}$**, E = -450.5031219 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.137588	1.423380	-0.759689
2	1	0	0.369162	0.711650	-1.555466
3	1	0	0.041636	2.418368	-1.207155
4	6	0	1.264174	1.445714	0.273716
5	1	0	2.203424	1.744564	-0.210877

6	1	0	1.042004	2.167171	1.062750
7	7	0	1.417898	0.155158	0.967441
8	7	0	1.864377	-0.760363	0.257959
9	7	0	2.281476	-1.693330	-0.277479
10	7	0	-1.129073	1.019601	-0.189775
11	1	0	-1.558951	1.628668	0.490725
12	6	0	-1.506987	-0.303479	-0.185239
13	6	0	-2.700268	-0.621374	0.688183
14	1	0	-3.340574	0.246867	0.859908
15	1	0	-3.277632	-1.417253	0.217837
16	1	0	-2.333741	-0.986835	1.651782
17	8	0	-0.919389	-1.153263	-0.839794

g⁻gg, E = -450.5066436 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.356563	-1.597626	0.571731
2	1	0	0.840004	-1.879913	1.509542
3	1	0	-0.160587	-2.470533	0.161637
4	6	0	1.410910	-1.135137	-0.432497
5	1	0	2.163308	-1.913603	-0.567864
6	1	0	0.940720	-0.918904	-1.396114
7	7	0	2.141776	0.049684	0.065690
8	7	0	1.553171	1.130473	-0.071840
9	7	0	1.141911	2.207702	-0.160757
10	7	0	-0.616299	-0.563844	0.865057
11	1	0	-0.497846	-0.002583	1.694461
12	6	0	-1.510956	-0.151130	-0.088468
13	6	0	-2.325833	1.067160	0.279939
14	1	0	-2.499031	1.141254	1.355983
15	1	0	-1.784170	1.959748	-0.048327
16	1	0	-3.279269	1.025442	-0.245889
17	8	0	-1.606393	-0.726077	-1.166838

g⁻gg⁻, E = -450.5039351 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.651730	-1.607246	0.075627
2	1	0	-0.473211	-1.730332	-0.994304
3	1	0	-0.754712	-2.597583	0.533942
4	6	0	-1.940683	-0.818009	0.289103
5	1	0	-2.789955	-1.386423	-0.094195
6	1	0	-2.104195	-0.632046	1.359506
7	7	0	-1.952238	0.451790	-0.453919
8	7	0	-1.165480	1.323532	-0.060823
9	7	0	-0.521348	2.248243	0.198662
10	7	0	0.502531	-0.923656	0.616931
11	1	0	0.615555	-0.866676	1.617816
12	6	0	1.439989	-0.311029	-0.183881
13	6	0	2.506582	0.451975	0.567683
14	1	0	2.678495	0.060267	1.573101

15	1	0	3.433187	0.418023	-0.005042
16	1	0	2.184682	1.494734	0.645697
17	8	0	1.380118	-0.344184	-1.404208

CH_2Cl_2

1,2-Diazidoethane

aaa, E = -406.1988205 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.395994	0.646080	0.111031
2	1	0	-1.057577	0.679248	0.982827
3	1	0	-0.995939	0.721836	-0.801326
4	6	0	0.395994	-0.646080	0.111031
5	1	0	0.995939	-0.721836	-0.801326
6	1	0	1.057577	-0.679248	0.982827
7	7	0	0.593820	1.742538	0.179267
8	7	0	0.145301	2.870464	-0.053443
9	7	0	-0.145301	3.970406	-0.246921
10	7	0	-0.593820	-1.742538	0.179267
11	7	0	-0.145301	-2.870464	-0.053443
12	7	0	0.145301	-3.970406	-0.246921

aag, E = -406.1991311 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.398356	0.007714	0.228785
2	1	0	-0.533379	0.047227	1.314644
3	1	0	-0.103060	-1.007436	-0.060907
4	6	0	0.659198	1.014725	-0.195897
5	1	0	0.774638	1.009068	-1.284871
6	1	0	0.376706	2.016129	0.126406
7	7	0	-1.646427	0.386318	-0.470415
8	7	0	-2.664951	-0.185860	-0.065668
9	7	0	-3.683893	-0.648913	0.215533
10	7	0	1.946607	0.725869	0.468501
11	7	0	2.542170	-0.276977	0.052535
12	7	0	3.209357	-1.171811	-0.242286

gag, E = -406.1995517 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.750319	0.141506	-0.704163
2	1	0	-1.026265	0.688438	-1.605080
3	1	0	-1.034882	0.734882	0.172493
4	6	0	0.750319	-0.141506	-0.704163

5	1	0	1.034882	-0.734882	0.172493
6	1	0	1.026265	-0.688438	-1.605080
7	7	0	-1.520914	-1.119238	-0.741309
8	7	0	-1.520914	-1.764699	0.315806
9	7	0	-1.617759	-2.458214	1.233727
10	7	0	1.520914	1.119238	-0.741309
11	7	0	1.520914	1.764699	0.315806
12	7	0	1.617759	2.458214	1.233727

gag–, E = -406.1994448 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.365666	-0.614941	0.265941
2	1	0	0.365881	-0.619839	1.356584
3	1	0	1.401559	-0.621581	-0.088814
4	6	0	-0.365666	0.614941	-0.265941
5	1	0	-0.365881	0.619839	-1.356584
6	1	0	-1.401559	0.621581	0.088814
7	7	0	-0.335251	-1.853474	-0.133124
8	7	0	-0.247816	-2.142023	-1.334330
9	7	0	-0.239151	-2.536471	-2.419288
10	7	0	0.335251	1.853474	0.133124
11	7	0	0.247816	2.142023	1.334330
12	7	0	0.239151	2.536471	2.419288

aga, E = -406.2006827 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.288768	-0.697219	1.035275
2	1	0	-0.003550	-1.207899	1.961217
3	1	0	-1.380992	-0.648297	0.970503
4	6	0	0.288768	0.697219	1.035275
5	1	0	0.003550	1.207899	1.961217
6	1	0	1.380992	0.648297	0.970503
7	7	0	-0.268174	1.416312	-0.131240
8	7	0	0.288768	2.484392	-0.406323
9	7	0	0.268174	-1.416312	-0.131240
10	7	0	-0.288768	-2.484392	-0.406323
11	7	0	0.721701	3.491369	-0.768633
12	7	0	-0.721701	-3.491369	-0.768633

agg, E = -406.2007007 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.891090	1.389787	0.082519
2	1	0	-1.535022	1.760104	0.887900
3	1	0	-0.671297	2.209880	-0.600402
4	6	0	0.391879	0.845860	0.679362
5	1	0	0.860698	1.623332	1.292855

6	1	0	0.182623	-0.021970	1.316310
7	7	0	1.287338	0.467156	-0.433910
8	7	0	2.199598	-0.311519	-0.135613
9	7	0	-1.611540	0.385632	-0.729759
10	7	0	-1.985166	-0.619345	-0.113200
11	7	0	3.091741	-1.028895	0.010973
12	7	0	-2.387933	-1.605204	0.334660

agg⁻, E = -406.202335 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.017453	1.396852	0.247848
2	1	0	1.389522	2.377229	-0.050345
3	1	0	1.168702	1.271595	1.325378
4	6	0	-0.456384	1.296915	-0.088712
5	1	0	-1.001604	2.107587	0.408089
6	1	0	-0.599100	1.368748	-1.171951
7	7	0	-0.928756	-0.015622	0.405874
8	7	0	-2.061732	-0.344712	0.039294
9	7	0	1.824653	0.416906	-0.505976
10	7	0	1.781861	-0.750872	-0.096160
11	7	0	-3.102846	-0.763517	-0.230603
12	7	0	1.869116	-1.869006	0.178144

ggg, E = -406.2009138 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.711404	-0.272072	1.039564
2	1	0	-0.856037	-0.894550	1.930101
3	1	0	-1.440013	0.539315	1.064643
4	6	0	0.711404	0.272072	1.039564
5	1	0	0.856037	0.894550	1.930101
6	1	0	1.440013	-0.539315	1.064643
7	7	0	1.028083	1.035689	-0.185256
8	7	0	0.299543	2.011021	-0.404336
9	7	0	-1.028083	-1.035689	-0.185256
10	7	0	-0.299543	-2.011021	-0.404336
11	7	0	-0.299543	2.943581	-0.729284
12	7	0	0.299543	-2.943581	-0.729284

g⁻gg⁻, E = -406.2024919 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.337587	1.181686	0.052534
2	1	0	1.996901	1.884744	-0.458288
3	1	0	1.630185	1.116051	1.105480
4	6	0	-0.100964	1.665902	-0.064580
5	1	0	-0.184243	2.656553	0.386898
6	1	0	-0.395625	1.724221	-1.116483

7	7	0	-1.009817	0.774607	0.689459
8	7	0	-1.642843	-0.048082	0.016135
9	7	0	1.534244	-0.116549	-0.621685
10	7	0	1.111003	-1.110543	-0.015348
11	7	0	-2.289206	-0.865481	-0.480624
12	7	0	0.801339	-2.129252	0.434159

ggg^{-}, E = -406.202462 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.447556	1.487767	-0.385723
2	1	0	-1.232987	2.132593	0.025222
3	1	0	-0.017667	1.961751	-1.267376
4	6	0	0.632579	1.261974	0.663102
5	1	0	1.040081	2.224821	0.973825
6	1	0	0.221398	0.758808	1.546738
7	7	0	1.772887	0.496968	0.122207
8	7	0	1.578500	-0.715185	-0.040558
9	7	0	-1.020266	0.211431	-0.867916
10	7	0	-1.697341	-0.411660	-0.040058
11	7	0	1.559537	-1.856493	-0.217391
12	7	0	-2.353455	-1.093120	0.623334

2-Azidoethanamine

aaa, E = -298.1491479 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.497475	0.745199	0.000000
2	1	0	-1.945644	0.280350	0.882272
3	1	0	-1.945644	0.280350	-0.882272
4	6	0	0.000000	0.462392	0.000000
5	1	0	0.467599	0.895570	-0.892147
6	1	0	0.467599	0.895570	0.892147
7	7	0	0.183365	-1.010877	0.000000
8	7	0	1.356517	-1.395607	0.000000
9	7	0	2.405326	-1.880203	0.000000
10	7	0	-1.830167	2.166389	0.000000
11	1	0	-1.432171	2.622353	0.815367
12	1	0	-1.432171	2.622353	-0.815367

aag, E = -298.1488009 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.578840	0.494193	-0.046904
2	1	0	1.585238	1.189257	0.803174
3	1	0	1.559594	1.087176	-0.964555
4	6	0	0.317121	-0.347028	0.023946

5	1	0	0.222712	-0.958590	-0.879055
6	1	0	0.348839	-1.007194	0.898843
7	7	0	-0.835753	0.578788	0.144627
8	7	0	-1.945954	0.055824	0.009787
9	7	0	-3.036517	-0.310495	-0.094436
10	7	0	2.738771	-0.397472	-0.093763
11	1	0	3.575563	0.137171	-0.303041
12	1	0	2.888470	-0.817326	0.818879

gaa, E = -298.149675 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.196130	-0.351112	-0.383638
2	1	0	1.211413	-0.176879	-1.462921
3	1	0	0.677017	-1.299625	-0.212455
4	6	0	0.413076	0.780080	0.284724
5	1	0	0.365572	0.624738	1.369339
6	1	0	0.890888	1.741366	0.091044
7	7	0	-0.957237	0.904696	-0.269284
8	7	0	-1.717566	-0.035664	-0.012639
9	7	0	-2.532875	-0.836613	0.159625
10	7	0	2.569799	-0.487162	0.091398
11	1	0	3.083153	0.374440	-0.068202
12	1	0	2.581872	-0.654652	1.092985

gag, E = -298.1491991 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.186362	-0.369221	0.328003
2	1	0	-1.157814	-0.278676	1.422000
3	1	0	-0.699408	-1.311613	0.058938
4	6	0	-0.403406	0.789937	-0.275706
5	1	0	-0.346784	0.683741	-1.364063
6	1	0	-0.884590	1.740513	-0.041490
7	7	0	0.958126	0.892111	0.302232
8	7	0	1.719611	-0.039905	0.019930
9	7	0	2.534327	-0.837176	-0.169860
10	7	0	-2.537544	-0.375762	-0.235319
11	1	0	-3.020042	-1.226306	0.036940
12	1	0	-3.074398	0.393164	0.155018

gag^{-}, E = -298.1491328 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.204808	-0.306163	-0.392588
2	1	0	1.268485	-0.096209	-1.463234
3	1	0	0.672104	-1.260243	-0.270390
4	6	0	0.401722	0.803570	0.273940
5	1	0	0.354984	0.647732	1.358528

6	1	0	0.863544	1.770752	0.079814
7	7	0	-0.970102	0.895292	-0.279506
8	7	0	-1.713480	-0.055719	-0.012987
9	7	0	-2.515578	-0.867882	0.167767
10	7	0	2.558062	-0.316794	0.164815
11	1	0	2.540050	-0.695126	1.107305
12	1	0	3.149332	-0.935623	-0.380759

aga, E = -298.1508327 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.756393	0.481560	-0.164318
2	1	0	-1.842999	0.671837	-1.238082
3	1	0	-2.433566	1.171787	0.347231
4	6	0	-0.335966	0.805340	0.274869
5	1	0	-0.100291	1.857710	0.078737
6	1	0	-0.214977	0.602563	1.345643
7	7	0	0.580992	-0.063053	-0.506711
8	7	0	1.738732	-0.128653	-0.083781
9	7	0	2.847480	-0.267542	0.209079
10	7	0	-2.190299	-0.886567	0.100948
11	1	0	-1.538103	-1.533612	-0.333228
12	1	0	-2.154251	-1.070980	1.099644

agg, E = -298.1508842 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.745881	0.487190	0.168493
2	1	0	1.832861	0.637624	1.253560
3	1	0	2.415381	1.198451	-0.323345
4	6	0	0.329392	0.814316	-0.251796
5	1	0	0.080459	1.850157	0.001672
6	1	0	0.216119	0.660096	-1.330154
7	7	0	-0.576318	-0.106304	0.485130
8	7	0	-1.742211	-0.137722	0.080909
9	7	0	-2.855988	-0.255059	-0.201867
10	7	0	2.095432	-0.864869	-0.267917
11	1	0	3.051416	-1.075838	0.002308
12	1	0	1.505721	-1.531853	0.221990

gga, E = -298.1508857 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.317476	-0.043699	0.678770
2	1	0	0.707082	-0.688939	1.319801
3	1	0	2.079136	0.413316	1.318331
4	6	0	0.444383	1.073664	0.113913
5	1	0	0.025899	1.685692	0.921870
6	1	0	1.025198	1.714917	-0.550533

7	7	0	-0.653252	0.538101	-0.732701
8	7	0	-1.528318	-0.085316	-0.121356
9	7	0	-2.413669	-0.678834	0.325700
10	7	0	1.981864	-0.878222	-0.318018
11	1	0	1.290232	-1.270470	-0.950543
12	1	0	2.594927	-0.304411	-0.890395

ggg, E = -298.1508233 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.320887	-0.012216	0.662417
2	1	0	0.716045	-0.657429	1.317473
3	1	0	2.089785	0.455638	1.284543
4	6	0	0.437081	1.088669	0.103548
5	1	0	0.015933	1.695653	0.912173
6	1	0	1.009275	1.727963	-0.568252
7	7	0	-0.661768	0.535003	-0.732779
8	7	0	-1.521292	-0.099473	-0.110763
9	7	0	-2.392442	-0.705627	0.347074
10	7	0	1.975459	-0.732902	-0.429293
11	1	0	2.550210	-1.480221	-0.051696
12	1	0	1.271234	-1.179335	-1.009704

ggg^{-}, E = -298.1493907 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.280308	-0.056434	0.631425
2	1	0	0.672578	-0.619467	1.347303
3	1	0	2.151871	0.328816	1.179998
4	6	0	0.497393	1.152096	0.142602
5	1	0	0.228561	1.786076	0.994886
6	1	0	1.093243	1.745328	-0.552939
7	7	0	-0.728444	0.796436	-0.613745
8	7	0	-1.440279	-0.066801	-0.094452
9	7	0	-2.187686	-0.866798	0.276618
10	7	0	1.616355	-0.947116	-0.477905
11	1	0	2.243730	-0.471537	-1.120439
12	1	0	2.124185	-1.753229	-0.126582

g*$^{-}$*ga, E = -298.1502543 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.682521	-0.123308	-0.122471
2	1	0	1.908780	-0.365460	-1.164383
3	1	0	2.577679	-0.343585	0.468947
4	6	0	0.572305	-1.050722	0.368301
5	1	0	0.879552	-2.092678	0.260924
6	1	0	0.346508	-0.857579	1.423756
7	7	0	-0.661856	-0.910889	-0.443190

8	7	0	-1.451491	-0.033824	-0.077330
9	7	0	-2.289956	0.721454	0.172953
10	7	0	1.402215	1.305281	-0.037247
11	1	0	0.654828	1.566248	-0.671500
12	1	0	1.111321	1.563090	0.900976

g⁻gg, E = -298.1504465 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.673695	-0.125480	-0.097829
2	1	0	1.960660	-0.368974	-1.129035
3	1	0	2.542659	-0.302691	0.543089
4	6	0	0.573932	-1.075935	0.346249
5	1	0	0.878105	-2.111802	0.189085
6	1	0	0.345266	-0.923430	1.406138
7	7	0	-0.654856	-0.893381	-0.466488
8	7	0	-1.440975	-0.026104	-0.069810
9	7	0	-2.275972	0.725989	0.198996
10	7	0	1.238089	1.262895	0.072221
11	1	0	2.044624	1.878722	0.080999
12	1	0	0.678923	1.550862	-0.725240

g⁻gg⁻, E = -298.1510454 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.615678	-0.111372	-0.217111
2	1	0	1.670679	-0.267608	-1.297519
3	1	0	2.597013	-0.362104	0.211327
4	6	0	0.594649	-1.078472	0.360562
5	1	0	0.930756	-2.106857	0.223839
6	1	0	0.459327	-0.898347	1.434358
7	7	0	-0.709207	-0.997682	-0.332107
8	7	0	-1.419141	-0.021044	-0.069314
9	7	0	-2.211511	0.803655	0.094987
10	7	0	1.193616	1.266972	0.029888
11	1	0	1.335739	1.500926	1.008519
12	1	0	1.768223	1.909745	-0.505412

2-Azidoethylammonium ion

aa, E = -298.5865044 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.477465	0.532445	-0.043634
2	1	0	1.535983	1.222608	0.796773
3	1	0	1.482651	1.089359	-0.979076
4	6	0	0.246114	-0.350368	0.060585
5	1	0	0.188328	-1.031409	-0.796120

6	1	0	0.266296	-0.936973	0.986354
7	7	0	-0.890463	0.585832	0.065446
8	7	0	-2.004945	0.048082	-0.001288
9	7	0	-3.096112	-0.316907	-0.057731
10	7	0	2.718202	-0.303506	-0.017120
11	1	0	2.811590	-0.819116	0.861398
12	1	0	2.731213	-0.987129	-0.778028
13	1	0	3.555686	0.275696	-0.118156

ag, E = -298.5861613 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.150524	-0.309287	-0.404845
2	1	0	1.234046	-0.087751	-1.467749
3	1	0	0.730189	-1.305900	-0.270335
4	6	0	0.317797	0.752469	0.306014
5	1	0	0.225737	0.529336	1.374744
6	1	0	0.771392	1.737352	0.190033
7	7	0	-1.004483	0.846446	-0.332019
8	7	0	-1.804789	-0.049663	-0.018104
9	7	0	-2.654475	-0.800574	0.187467
10	7	0	2.542301	-0.346752	0.149929
11	1	0	3.028875	0.543371	0.013727
12	1	0	2.548596	-0.552551	1.152315
13	1	0	3.101360	-1.069133	-0.310662

ga, E = -298.5922117 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.672371	0.589770	-0.224245
2	1	0	-1.740339	0.663552	-1.308716
3	1	0	-2.382414	1.272006	0.240442
4	6	0	-0.261283	0.850846	0.254790
5	1	0	0.047809	1.842480	-0.088478
6	1	0	-0.206200	0.816755	1.348671
7	7	0	0.570025	-0.213191	-0.344033
8	7	0	1.776364	-0.160456	-0.065543
9	7	0	2.911775	-0.217320	0.116145
10	7	0	-2.066028	-0.806295	0.141297
11	1	0	-1.361690	-1.465408	-0.206868
12	1	0	-2.128624	-0.929615	1.154768
13	1	0	-2.971570	-1.062629	-0.258154

gg, E = -298.5908914 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.313064	0.190958	0.714875
2	1	0	0.803022	-0.410531	1.467724
3	1	0	2.101306	0.776516	1.187325

4	6	0	0.340921	1.077396	-0.045953
5	1	0	-0.146588	1.759067	0.656247
6	1	0	0.860648	1.670468	-0.799747
7	7	0	-0.638983	0.251494	-0.782699
8	7	0	-1.604356	-0.138105	-0.103972
9	7	0	-2.555062	-0.550021	0.399458
10	7	0	1.958838	-0.764143	-0.239342
11	1	0	1.240941	-1.257064	-0.780435
12	1	0	2.566936	-0.281024	-0.905091
13	1	0	2.526760	-1.462126	0.246325

2-Azidoethanol

aaa, E = -318.0004202 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.583286	0.475138	-0.082319
2	1	0	-1.551842	0.977690	-1.054534
3	1	0	-1.630337	1.233029	0.707322
4	6	0	-0.332873	-0.360464	0.099127
5	1	0	-0.391184	-0.919129	1.038879
6	1	0	-0.225037	-1.063622	-0.732764
7	7	0	0.810730	0.579032	0.138313
8	7	0	1.923217	0.061515	-0.000657
9	7	0	3.015028	-0.296482	-0.113406
10	1	0	-3.477512	0.071303	-0.221260
11	8	0	-2.683744	-0.424471	-0.001029

aag, E = -318.0005807 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.592385	0.491686	-0.057252
2	1	0	-1.565255	1.064663	-0.984913
3	1	0	-1.644353	1.190914	0.784299
4	6	0	-0.335391	-0.354671	0.060404
5	1	0	-0.372563	-0.968912	0.967562
6	1	0	-0.245073	-1.010199	-0.811701
7	7	0	0.811989	0.578845	0.134994
8	7	0	1.923613	0.056469	0.005771
9	7	0	3.014682	-0.306765	-0.097439
10	1	0	-2.845482	-0.770479	0.724284
11	8	0	-2.751575	-0.328490	-0.125215

gaa, E = -318.0007332 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.220647	-0.343722	0.361980
2	1	0	-1.290878	-0.170755	1.440999

3	1	0	-0.716576	-1.302783	0.190658
4	6	0	-0.420883	0.781326	-0.273251
5	1	0	-0.352527	0.635601	-1.356374
6	1	0	-0.896797	1.740569	-0.073405
7	7	0	0.929964	0.870622	0.323900
8	7	0	1.705298	-0.044104	0.019728
9	7	0	2.535478	-0.819470	-0.189236
10	1	0	-3.055391	-0.963090	0.211704
11	8	0	-2.504228	-0.326812	-0.253337

gag, E = -318.0008458 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.223562	-0.334771	-0.391427
2	1	0	1.288162	-0.126315	-1.460240
3	1	0	0.720098	-1.299636	-0.256139
4	6	0	0.426939	0.771282	0.292545
5	1	0	0.363637	0.592149	1.372470
6	1	0	0.906381	1.734933	0.124184
7	7	0	-0.929881	0.887263	-0.286616
8	7	0	-1.704229	-0.038866	-0.015625
9	7	0	-2.534186	-0.821468	0.166419
10	1	0	2.524181	-0.657302	1.014805
11	8	0	2.559075	-0.381425	0.093619

***gag*$^-$**, E = -318.0008896 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.213862	-0.369840	0.357731
2	1	0	-1.257693	-0.213445	1.440883
3	1	0	-0.717540	-1.323863	0.166333
4	6	0	-0.427816	0.765792	-0.289090
5	1	0	-0.362169	0.611522	-1.371171
6	1	0	-0.913272	1.724030	-0.099857
7	7	0	0.922858	0.884586	0.304654
8	7	0	1.707053	-0.029175	0.020223
9	7	0	2.543778	-0.802064	-0.171601
10	1	0	-3.006819	0.305410	0.043339
11	8	0	-2.513533	-0.481599	-0.208038

aga, E = -318.0016756 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.743486	0.453821	0.165647
2	1	0	1.801413	0.571541	1.252959
3	1	0	2.419074	1.177040	-0.305681
4	6	0	0.337242	0.748730	-0.293408
5	1	0	0.123848	1.815418	-0.165375
6	1	0	0.233603	0.484151	-1.351293

7	7	0	-0.601656	-0.048591	0.530694
8	7	0	-1.753127	-0.126251	0.093110
9	7	0	-2.858547	-0.273874	-0.207170
10	1	0	2.885262	-1.116740	0.220834
11	8	0	2.068218	-0.875713	-0.225164

agg, E = -318.0013071 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.753406	0.452941	-0.159117
2	1	0	-1.827870	0.630486	-1.233277
3	1	0	-2.433227	1.141944	0.355783
4	6	0	-0.341624	0.745943	0.305167
5	1	0	-0.135800	1.816782	0.192550
6	1	0	-0.224514	0.475172	1.361451
7	7	0	0.598523	-0.036412	-0.528707
8	7	0	1.749944	-0.120200	-0.091798
9	7	0	2.855554	-0.272179	0.205565
10	1	0	-2.121934	-1.064144	0.992810
11	8	0	-2.139328	-0.899001	0.044871

agg^{-}, E = -318.0039706 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.772387	0.427884	0.149430
2	1	0	1.894233	0.572577	1.229093
3	1	0	2.487852	1.064958	-0.373240
4	6	0	0.367720	0.820886	-0.255344
5	1	0	0.179157	1.872896	-0.015978
6	1	0	0.228609	0.654322	-1.328437
7	7	0	-0.555902	-0.047633	0.517575
8	7	0	-1.710733	-0.114236	0.084115
9	7	0	-2.816259	-0.253211	-0.217083
10	1	0	1.394961	-1.460422	0.195494
11	8	0	2.069351	-0.911424	-0.220462

gga, E = -318.0016592 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.304772	-0.115357	0.628581
2	1	0	0.683501	-0.834900	1.176165
3	1	0	2.081076	0.255653	1.308812
4	6	0	0.463437	1.062990	0.186323
5	1	0	0.106769	1.609619	1.066539
6	1	0	1.057105	1.736556	-0.431219
7	7	0	-0.685358	0.665297	-0.661457
8	7	0	-1.509766	-0.074191	-0.114521
9	7	0	-2.351651	-0.764767	0.272669
10	1	0	2.284186	-1.538934	-0.255538

11	8	0	1.875692	-0.712271	-0.528877

ggg, E = -318.0018435 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.303060	-0.124355	0.633460
2	1	0	0.687379	-0.773535	1.260870
3	1	0	2.143315	0.234957	1.240084
4	6	0	0.499365	1.082543	0.177051
5	1	0	0.181079	1.659373	1.053697
6	1	0	1.102176	1.729220	-0.462055
7	7	0	-0.676135	0.717514	-0.646318
8	7	0	-1.478260	-0.053878	-0.109947
9	7	0	-2.304202	-0.766814	0.270585
10	1	0	2.305285	-0.390530	-1.007046
11	8	0	1.747048	-0.935796	-0.443607

ggg^{-}, E = -318.0034583 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.346096	-0.058817	0.658595
2	1	0	0.750179	-0.722928	1.298001
3	1	0	2.139165	0.381411	1.266602
4	6	0	0.467936	1.048792	0.105075
5	1	0	0.050683	1.653261	0.918137
6	1	0	1.045656	1.687832	-0.562090
7	7	0	-0.621996	0.491441	-0.737466
8	7	0	-1.523508	-0.081261	-0.111849
9	7	0	-2.432454	-0.626316	0.347318
10	1	0	1.291061	-1.098383	-0.970215
11	8	0	1.985596	-0.791011	-0.377309

g^{-}***ga***, E = -318.0038721 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.607016	-0.017422	-0.205679
2	1	0	1.686623	-0.134930	-1.291564
3	1	0	2.594772	-0.167440	0.246640
4	6	0	0.655014	-1.056400	0.344579
5	1	0	1.051936	-2.055496	0.164126
6	1	0	0.526150	-0.914691	1.423388
7	7	0	-0.656818	-1.021348	-0.336317
8	7	0	-1.386822	-0.060472	-0.065220
9	7	0	-2.187710	0.754761	0.100979
10	1	0	1.599450	1.926140	-0.320756
11	8	0	1.073543	1.259846	0.131083

g^{-}***gg***, E = -318.0034179 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.600962	-0.010803	-0.233079
2	1	0	1.659469	-0.149080	-1.313796
3	1	0	2.600650	-0.146841	0.196198
4	6	0	0.660964	-1.046295	0.359466
5	1	0	1.062595	-2.048096	0.201032
6	1	0	0.540094	-0.884538	1.437524
7	7	0	-0.658677	-1.036358	-0.304592
8	7	0	-1.386373	-0.066658	-0.060877
9	7	0	-2.187293	0.752563	0.087292
10	1	0	1.215953	1.514789	0.906750
11	8	0	1.122011	1.313691	-0.029848

Protonated 2-azidoethanol

aaa, E = -318.3826646 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.430642	0.510843	-0.183859
2	1	0	1.543483	1.356913	0.488913
3	1	0	1.397615	0.837636	-1.219282
4	6	0	0.266546	-0.381771	0.200254
5	1	0	0.116831	-1.166319	-0.547576
6	1	0	0.429560	-0.839129	1.181968
7	7	0	-0.870651	0.551985	0.246377
8	7	0	-1.976393	0.045308	0.005092
9	7	0	-3.058954	-0.288675	-0.197384
10	1	0	2.976617	-0.453234	0.839736
11	1	0	2.815440	-0.994773	-0.644034
12	8	0	2.734914	-0.209482	-0.072086

aag, E = -318.3831717 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.446315	0.527605	0.103099
2	1	0	-1.554093	1.265325	-0.688556
3	1	0	-1.454620	0.987144	1.087059
4	6	0	-0.259573	-0.388393	-0.102208
5	1	0	-0.137848	-1.048634	0.760602
6	1	0	-0.385316	-0.989971	-1.008668
7	7	0	0.871609	0.541606	-0.249451
8	7	0	1.983875	0.049325	-0.009548
9	7	0	3.071787	-0.275447	0.179835
10	1	0	-3.450283	0.093295	0.485962
11	1	0	-2.911528	-0.653636	-0.801123
12	8	0	-2.670235	-0.337147	0.089190

gaa, E = -318.3826259 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.150910	-0.290268	-0.428297
2	1	0	1.293606	-0.004239	-1.467050
3	1	0	0.763302	-1.303431	-0.354062
4	6	0	0.331611	0.725801	0.351132
5	1	0	0.222180	0.428049	1.398553
6	1	0	0.786340	1.715132	0.302849
7	7	0	-0.971447	0.837638	-0.322919
8	7	0	-1.797534	-0.041887	-0.021289
9	7	0	-2.669130	-0.769525	0.170809
10	1	0	3.112133	0.361548	-0.060834
11	1	0	2.607782	-0.664115	1.042786
12	8	0	2.548289	-0.416216	0.101818

gag, E = -318.3830431 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.148431	-0.269522	0.435074
2	1	0	-1.320907	0.004887	1.473304
3	1	0	-0.742411	-1.274222	0.346680
4	6	0	-0.328379	0.757039	-0.324480
5	1	0	-0.243336	0.480054	-1.378796
6	1	0	-0.769996	1.750004	-0.242424
7	7	0	0.985187	0.842356	0.333861
8	7	0	1.788004	-0.053183	0.017261
9	7	0	2.639223	-0.800978	-0.189069
10	1	0	-2.977785	-1.182673	0.009624
11	1	0	-3.068686	0.392283	-0.088881
12	8	0	-2.487864	-0.376600	-0.239680

gag^{-}, E = -318.383147 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.182077	-0.263462	-0.448402
2	1	0	1.354427	0.098567	-1.458418
3	1	0	0.824121	-1.291107	-0.445830
4	6	0	0.321791	0.691858	0.357340
5	1	0	0.202233	0.345324	1.388303
6	1	0	0.771468	1.683794	0.359025
7	7	0	-0.971305	0.812386	-0.332913
8	7	0	-1.815157	-0.047209	-0.026028
9	7	0	-2.700684	-0.756434	0.170646
10	1	0	2.600045	-0.778800	1.006406
11	1	0	3.248967	-0.576687	-0.422205
12	8	0	2.548195	-0.264084	0.179645

aga, E = -318.3907334 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.736644	0.537030	-0.159023
2	1	0	-1.922700	0.646185	-1.223765
3	1	0	-2.509064	1.017741	0.434542
4	6	0	-0.326963	0.921801	0.230708
5	1	0	-0.105800	1.914312	-0.171170
6	1	0	-0.200656	0.924461	1.317302
7	7	0	0.504910	-0.128246	-0.395761
8	7	0	1.703213	-0.127567	-0.067610
9	7	0	2.827652	-0.214805	0.150434
10	1	0	-0.981329	-1.321382	-0.118403
11	1	0	-2.136014	-1.168858	0.977925
12	8	0	-1.876652	-0.933890	0.068002

agg, E = -318.3919006 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.733114	0.541510	-0.162755
2	1	0	-1.913159	0.592894	-1.234560
3	1	0	-2.490183	1.065109	0.413223
4	6	0	-0.321481	0.922240	0.212195
5	1	0	-0.096449	1.907795	-0.203505
6	1	0	-0.200288	0.937691	1.299017
7	7	0	0.507160	-0.140794	-0.398234
8	7	0	1.706015	-0.133272	-0.071421
9	7	0	2.830642	-0.218368	0.146787
10	1	0	-2.593731	-1.364468	-0.160447
11	1	0	-0.985450	-1.319489	-0.040692
12	8	0	-1.837485	-0.894375	0.236299

***agg*$^-$**, E = -318.3868806 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.653350	0.589146	-0.210592
2	1	0	-1.715913	0.633151	-1.294624
3	1	0	-2.358520	1.264187	0.269191
4	6	0	-0.251684	0.769627	0.295234
5	1	0	0.014909	1.814602	0.096984
6	1	0	-0.200960	0.603261	1.377726
7	7	0	0.616400	-0.161171	-0.439890
8	7	0	1.803287	-0.150838	-0.081464
9	7	0	2.926723	-0.244977	0.153025
10	1	0	-2.104913	-1.010518	1.059451
11	1	0	-2.954959	-1.040739	-0.273083
12	8	0	-2.084289	-0.814710	0.104351

gga, E = -318.3894441 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.468326	0.456055	0.576008
2	1	0	1.113423	0.222847	1.576427
3	1	0	2.368770	1.064305	0.602083
4	6	0	0.373696	0.978791	-0.334543
5	1	0	-0.139051	1.814915	0.146241
6	1	0	0.782292	1.304089	-1.291560
7	7	0	-0.520563	-0.168859	-0.616480
8	7	0	-1.624465	-0.151371	-0.041873
9	7	0	-2.677672	-0.237900	0.407858
10	1	0	1.043675	-1.288233	-0.313719
11	1	0	2.518845	-0.810031	-0.696607
12	8	0	1.877352	-0.876257	0.035226

ggg, E = -318.3903229 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.459322	0.418455	0.594441
2	1	0	1.096357	0.098336	1.569699
3	1	0	2.350417	1.035827	0.665535
4	6	0	0.373055	1.011988	-0.280045
5	1	0	-0.134721	1.813670	0.259977
6	1	0	0.796545	1.406061	-1.203772
7	7	0	-0.532737	-0.096544	-0.663192
8	7	0	-1.611371	-0.150800	-0.043512
9	7	0	-2.646271	-0.294270	0.434162
10	1	0	2.395365	-1.438908	0.382270
11	1	0	1.037626	-1.235129	-0.466843
12	8	0	1.874600	-0.808901	-0.148181

***ggg*⁻**, E = -318.3859741 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.264981	0.035635	0.728898
2	1	0	0.735627	-0.734594	1.285776
3	1	0	2.058658	0.485418	1.322830
4	6	0	0.349278	1.065245	0.113047
5	1	0	-0.077540	1.643120	0.940980
6	1	0	0.908035	1.754212	-0.520812
7	7	0	-0.687474	0.469130	-0.739823
8	7	0	-1.596996	-0.112700	-0.126635
9	7	0	-2.505156	-0.675364	0.304936
10	1	0	2.476633	-0.181435	-0.964053
11	1	0	2.440589	-1.489959	-0.076976
12	8	0	1.912478	-0.731188	-0.388596

***g*⁻*gg*⁻**, E = -318.3861194 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.626041	-0.234929	-0.170026
2	1	0	1.734406	-0.339714	-1.246180
3	1	0	2.572590	-0.369786	0.350032
4	6	0	0.514127	-1.092850	0.379183
5	1	0	0.841445	-2.129401	0.278781
6	1	0	0.344226	-0.893275	1.442160
7	7	0	-0.718652	-0.956089	-0.408265
8	7	0	-1.461805	-0.019992	-0.073037
9	7	0	-2.254116	0.790600	0.134173
10	1	0	1.393921	1.555951	0.903192
11	1	0	1.606034	1.809142	-0.644400
12	8	0	1.213548	1.204016	0.011421

N-(2-Azidoethyl)ethanamide

aag, E = -450.5121692 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.129870	0.944573	-0.537833
2	1	0	-0.153334	1.997041	-0.594885
3	1	0	0.197892	0.541686	-1.550808
4	6	0	-0.913722	0.164402	0.249464
5	1	0	-0.623020	-0.888773	0.309013
6	1	0	-1.007002	0.575923	1.260462
7	7	0	-2.197120	0.299911	-0.479473
8	7	0	-3.176767	-0.191411	0.090406
9	7	0	-4.165737	-0.607648	0.517347
10	7	0	1.431139	0.852656	0.092520
11	1	0	1.735619	1.595796	0.702842
12	6	0	2.222879	-0.242067	-0.061718
13	6	0	3.544249	-0.208830	0.669786
14	1	0	3.693560	0.707731	1.242490
15	1	0	3.590380	-1.066796	1.343617
16	1	0	4.348049	-0.311393	-0.062127
17	8	0	1.884700	-1.196780	-0.764298

gag, E = -450.5129271 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.100774	-0.751188	-0.678938
2	1	0	0.362923	-1.584618	-1.333356
3	1	0	0.350260	0.184583	-1.186873
4	6	0	0.877928	-0.851793	0.633713
5	1	0	0.577080	-0.045997	1.310388
6	1	0	0.689016	-1.811860	1.113854
7	7	0	2.338137	-0.806394	0.393643
8	7	0	2.773856	0.294166	0.031990
9	7	0	3.314979	1.259832	-0.298089
10	7	0	-1.328277	-0.776287	-0.442713
11	1	0	-1.827961	-1.648409	-0.529200

12	6	0	-1.994263	0.333297	-0.024129
13	6	0	-3.475654	0.164363	0.216395
14	1	0	-3.827900	-0.849474	0.020746
15	1	0	-3.691575	0.427263	1.253972
16	1	0	-4.013289	0.863468	-0.427393
17	8	0	-1.420266	1.412220	0.137724

***gag*⁻**, E = -450.5124298 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.162369	-0.352279	-0.513526
2	1	0	-0.079691	0.317241	-1.372478
3	1	0	-0.738289	-1.232375	-0.810190
4	6	0	-0.857920	0.381829	0.632777
5	1	0	-0.954852	-0.274812	1.504550
6	1	0	-0.282123	1.263268	0.910558
7	7	0	-2.186722	0.885671	0.218356
8	7	0	-3.043783	0.014818	0.025352
9	7	0	-3.938736	-0.687182	-0.177846
10	7	0	1.163612	-0.788771	-0.126390
11	1	0	1.292922	-1.729789	0.213302
12	6	0	2.216444	0.072449	-0.105782
13	6	0	3.533470	-0.506675	0.354538
14	1	0	3.468905	-1.564423	0.614111
15	1	0	4.267220	-0.375654	-0.443414
16	1	0	3.876574	0.057916	1.223972
17	8	0	2.101374	1.249366	-0.453094

agg, E = -450.5144087 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.231273	-1.454260	-0.442835
2	1	0	-0.084583	-1.940365	-1.368142
3	1	0	0.778300	-2.178307	0.164672
4	6	0	-0.982003	-0.979763	0.338374
5	1	0	-1.632137	-1.829211	0.575624
6	1	0	-0.662479	-0.494755	1.266076
7	7	0	-1.703644	-0.009163	-0.520196
8	7	0	-2.691048	0.520026	0.000096
9	7	0	-3.628987	1.082624	0.371096
10	7	0	1.124300	-0.364691	-0.781409
11	1	0	0.949411	0.150029	-1.631494
12	6	0	1.956822	0.181093	0.145215
13	6	0	2.712073	1.413368	-0.294263
14	1	0	2.593386	1.629024	-1.357252
15	1	0	2.350569	2.265638	0.286354
16	1	0	3.770545	1.274907	-0.067280
17	8	0	2.090456	-0.305144	1.270674

***agg*⁻**, E = -450.5127234 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.228111	1.571634	0.154075
2	1	0	0.364205	1.461829	1.230459
3	1	0	0.399115	2.617909	-0.116054
4	6	0	-1.191625	1.193925	-0.231797
5	1	0	-1.900230	1.844085	0.293747
6	1	0	-1.338860	1.306094	-1.312499
7	7	0	-1.403358	-0.219773	0.154933
8	7	0	-2.556911	-0.634175	0.006427
9	7	0	-3.591340	-1.139236	-0.090395
10	7	0	1.208471	0.728246	-0.495383
11	1	0	1.292092	0.776918	-1.500580
12	6	0	1.891808	-0.252665	0.156978
13	6	0	2.762692	-1.122335	-0.720991
14	1	0	2.873819	-0.732555	-1.734107
15	1	0	3.745816	-1.217002	-0.257321
16	1	0	2.314015	-2.117742	-0.769844
17	8	0	1.813259	-0.428541	1.373441

ggg, E = -450.5140946 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.143988	0.746113	0.910327
2	1	0	-0.834591	0.413217	1.689688
3	1	0	0.389598	1.625415	1.280263
4	6	0	-0.907022	1.138302	-0.350650
5	1	0	-1.588983	1.968520	-0.134727
6	1	0	-0.211281	1.441607	-1.131127
7	7	0	-1.659834	-0.006942	-0.916848
8	7	0	-2.609342	-0.404340	-0.232140
9	7	0	-3.521843	-0.869719	0.303309
10	7	0	0.813163	-0.314976	0.671591
11	1	0	0.525713	-1.271990	0.810072
12	6	0	1.989572	-0.072596	0.034215
13	6	0	2.838412	-1.285315	-0.266312
14	1	0	2.459454	-2.196299	0.199422
15	1	0	2.871062	-1.424606	-1.349665
16	1	0	3.855469	-1.095271	0.080713
17	8	0	2.339588	1.069027	-0.273938

***ggg*$^-$**, E = -450.5147428 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.139357	1.376725	-0.773022
2	1	0	0.382416	0.643469	-1.544991
3	1	0	0.023277	2.353392	-1.251668
4	6	0	1.267876	1.461369	0.250964
5	1	0	2.193031	1.782811	-0.242000
6	1	0	1.019261	2.179139	1.033311

7	7	0	1.478387	0.177719	0.956118
8	7	0	1.928781	-0.735883	0.254721
9	7	0	2.353721	-1.667371	-0.279087
10	7	0	-1.118356	0.982620	-0.175484
11	1	0	-1.636996	1.667445	0.354611
12	6	0	-1.540513	-0.311440	-0.152254
13	6	0	-2.813491	-0.565295	0.621451
14	1	0	-3.330449	0.352300	0.906917
15	1	0	-3.476092	-1.183187	0.013369
16	1	0	-2.560876	-1.126936	1.524350
17	8	0	-0.928834	-1.217022	-0.721326

g⁻gg, E = -450.5159553 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.310342	-1.572126	0.584769
2	1	0	0.770445	-1.843663	1.536403
3	1	0	-0.231092	-2.438833	0.193549
4	6	0	1.392554	-1.178270	-0.416418
5	1	0	2.105460	-1.995166	-0.532407
6	1	0	0.948176	-0.949428	-1.389053
7	7	0	2.179701	-0.021088	0.069120
8	7	0	1.646570	1.085202	-0.077684
9	7	0	1.289057	2.179864	-0.180557
10	7	0	-0.621060	-0.489136	0.835125
11	1	0	-0.562423	0.019698	1.704444
12	6	0	-1.550114	-0.114225	-0.084975
13	6	0	-2.379674	1.092813	0.281780
14	1	0	-2.395557	1.281335	1.356587
15	1	0	-1.955402	1.966950	-0.220846
16	1	0	-3.397358	0.948526	-0.081962
17	8	0	-1.672597	-0.705309	-1.159960

g⁻gg⁻, E = -450.5152881 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.642199	-1.625759	-0.057508
2	1	0	0.481025	-1.760339	1.012838
3	1	0	0.738785	-2.609063	-0.528037
4	6	0	1.926804	-0.836465	-0.287077
5	1	0	2.778920	-1.398365	0.097000
6	1	0	2.080846	-0.650141	-1.356412
7	7	0	1.931536	0.442335	0.453497
8	7	0	1.173988	1.324313	0.033096
9	7	0	0.551600	2.256281	-0.253134
10	7	0	-0.518177	-0.942232	-0.591089
11	1	0	-0.672572	-0.959638	-1.588936
12	6	0	-1.427415	-0.293409	0.191391
13	6	0	-2.528835	0.414435	-0.560839
14	1	0	-2.657357	0.040282	-1.578064
15	1	0	-3.462473	0.306557	-0.007906

16	1	0	-2.277054	1.478033	-0.605839
17	8	0	-1.332408	-0.245627	1.417871

DMSO

1,2-Diazidoethane

aaa, E = -406.1998083 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.397019	0.645456	0.118223
2	1	0	-1.058887	0.678661	0.989650
3	1	0	-0.995664	0.722040	-0.794703
4	6	0	0.397019	-0.645456	0.118223
5	1	0	0.995664	-0.722040	-0.794703
6	1	0	1.058887	-0.678661	0.989650
7	7	0	0.591534	1.743744	0.188424
8	7	0	0.144915	2.869392	-0.056660
9	7	0	-0.144915	3.967551	-0.260947
10	7	0	-0.591534	-1.743744	0.188424
11	7	0	-0.144915	-2.869392	-0.056660
12	7	0	0.144915	-3.967551	-0.260947

aag, E = -406.2001685 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.398810	0.003812	0.227352
2	1	0	-0.536052	0.042531	1.312753
3	1	0	-0.103684	-1.010728	-0.063588
4	6	0	0.657820	1.012248	-0.195944
5	1	0	0.775995	1.006552	-1.284461
6	1	0	0.374086	2.013183	0.126660
7	7	0	-1.647082	0.382457	-0.472944
8	7	0	-2.666699	-0.185193	-0.065934
9	7	0	-3.686619	-0.644621	0.217623
10	7	0	1.945077	0.724686	0.470493
11	7	0	2.544896	-0.274783	0.053438
12	7	0	3.215512	-1.166531	-0.242648

gag, E = -406.200656 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.750584	0.139708	-0.702491
2	1	0	-1.028264	0.686138	-1.603127
3	1	0	-1.037248	0.730491	0.174865
4	6	0	0.750584	-0.139708	-0.702491
5	1	0	1.037248	-0.730491	0.174865
6	1	0	1.028264	-0.686138	-1.603127

7	7	0	-1.517379	-1.123984	-0.741026
8	7	0	-1.517379	-1.770474	0.315090
9	7	0	-1.613746	-2.465121	1.232108
10	7	0	1.517379	1.123984	-0.741026
11	7	0	1.517379	1.770474	0.315090
12	7	0	1.613746	2.465121	1.232108

***gag*⁻**, E = -406.200527 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.365890	-0.615068	0.265311
2	1	0	0.365962	-0.621543	1.355825
3	1	0	1.401265	-0.622543	-0.090349
4	6	0	-0.365890	0.615068	-0.265311
5	1	0	-0.365962	0.621543	-1.355825
6	1	0	-1.401265	0.622543	0.090349
7	7	0	-0.335938	-1.853402	-0.135080
8	7	0	-0.247843	-2.143881	-1.335398
9	7	0	-0.238338	-2.540005	-2.419694
10	7	0	0.335938	1.853402	0.135080
11	7	0	0.247843	2.143881	1.335398
12	7	0	0.238338	2.540005	2.419694

aga, E = -406.2020134 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.319365	-0.683386	0.980156
2	1	0	-0.039522	-1.209715	1.898807
3	1	0	-1.409442	-0.589480	0.934032
4	6	0	0.319365	0.683386	0.980156
5	1	0	0.039522	1.209715	1.898807
6	1	0	1.409442	0.589480	0.934032
7	7	0	-0.183842	1.419322	-0.201262
8	7	0	0.319365	2.533048	-0.380998
9	7	0	0.183842	-1.419322	-0.201262
10	7	0	-0.319365	-2.533048	-0.380998
11	7	0	0.710947	3.582076	-0.662565
12	7	0	-0.710947	-3.582076	-0.662565

agg, E = -406.2020886 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.886729	1.388764	0.083279
2	1	0	-1.529893	1.758235	0.889216
3	1	0	-0.666863	2.209341	-0.598989
4	6	0	0.395338	0.842173	0.678791
5	1	0	0.868765	1.619955	1.287849
6	1	0	0.185853	-0.023366	1.318244
7	7	0	1.287334	0.456627	-0.436347

8	7	0	2.205231	-0.313775	-0.135662
9	7	0	-1.608809	0.385394	-0.730265
10	7	0	-1.993840	-0.614798	-0.113402
11	7	0	3.102005	-1.024828	0.013650
12	7	0	-2.407565	-1.595731	0.335064

***agg*⁻**, E = -406.2034749 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.001993	1.396135	0.262700
2	1	0	1.364282	2.384921	-0.018778
3	1	0	1.147077	1.256951	1.339109
4	6	0	-0.466887	1.283776	-0.089541
5	1	0	-1.027350	2.070997	0.427164
6	1	0	-0.603419	1.385116	-1.171015
7	7	0	-0.923929	-0.050954	0.360213
8	7	0	-2.075808	-0.354863	0.034770
9	7	0	1.827389	0.435401	-0.498457
10	7	0	1.806642	-0.734791	-0.096200
11	7	0	-3.132210	-0.753437	-0.204867
12	7	0	1.913456	-1.852422	0.173764

ggg, E = -406.2022304 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.709997	-0.275023	1.033179
2	1	0	-0.852167	-0.897218	1.923903
3	1	0	-1.442379	0.532831	1.055817
4	6	0	0.709997	0.275023	1.033179
5	1	0	0.852167	0.897218	1.923903
6	1	0	1.442379	-0.532831	1.055817
7	7	0	1.021140	1.042771	-0.191676
8	7	0	0.297692	2.023490	-0.401470
9	7	0	-1.021140	-1.042771	-0.191676
10	7	0	-0.297692	-2.023490	-0.401470
11	7	0	-0.297692	2.961264	-0.718110
12	7	0	0.297692	-2.961264	-0.718110

g⁻gg⁻, E = -406.2036376 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.358915	1.166081	0.054856
2	1	0	2.024869	1.861853	-0.456878
3	1	0	1.648858	1.100737	1.108374
4	6	0	-0.075120	1.660652	-0.068232
5	1	0	-0.151705	2.654059	0.378079
6	1	0	-0.368414	1.714932	-1.120487
7	7	0	-0.989951	0.776695	0.689319
8	7	0	-1.651499	-0.023775	0.017928

9	7	0	1.547425	-0.136892	-0.614421
10	7	0	1.098692	-1.124101	-0.016819
11	7	0	-2.320713	-0.823633	-0.477246
12	7	0	0.765135	-2.138576	0.425691

***ggg*⁻**, E = -406.2037057 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.446056	1.490206	-0.382137
2	1	0	-1.230602	2.132936	0.032802
3	1	0	-0.019668	1.966284	-1.264277
4	6	0	0.637135	1.262829	0.662860
5	1	0	1.047975	2.224924	0.970839
6	1	0	0.229608	0.760118	1.547984
7	7	0	1.773792	0.494137	0.116273
8	7	0	1.577969	-0.717771	-0.041247
9	7	0	-1.019273	0.213643	-0.865342
10	7	0	-1.699141	-0.409954	-0.040680
11	7	0	1.556084	-1.859842	-0.213691
12	7	0	-2.357115	-1.091996	0.620160

2-Azidoethanamine

aaa, E = -298.1505049 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.497112	0.746589	0.000000
2	1	0	-1.945582	0.282881	0.882783
3	1	0	-1.945582	0.282881	-0.882783
4	6	0	0.000000	0.463228	0.000000
5	1	0	0.468040	0.894980	-0.892214
6	1	0	0.468040	0.894980	0.892214
7	7	0	0.182133	-1.011090	0.000000
8	7	0	1.354338	-1.397524	0.000000
9	7	0	2.402595	-1.883262	0.000000
10	7	0	-1.826918	2.169118	0.000000
11	1	0	-1.423641	2.622342	0.814606
12	1	0	-1.423641	2.622342	-0.814606

aag, E = -298.1499706 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.579492	0.494280	-0.044383
2	1	0	1.585705	1.182899	0.810774
3	1	0	1.563214	1.093349	-0.958160
4	6	0	0.317355	-0.346765	0.018820
5	1	0	0.223506	-0.953574	-0.887409
6	1	0	0.345556	-1.010392	0.890935
7	7	0	-0.835993	0.579343	0.140136

8	7	0	-1.946302	0.056148	0.010140
9	7	0	-3.036957	-0.310951	-0.089950
10	7	0	2.739639	-0.397674	-0.093703
11	1	0	3.577749	0.141992	-0.285086
12	1	0	2.880478	-0.827418	0.815962

gaa, E = -298.1510172 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.196792	-0.351941	-0.384621
2	1	0	1.212649	-0.176292	-1.463676
3	1	0	0.678154	-1.300648	-0.213478
4	6	0	0.414317	0.778566	0.285048
5	1	0	0.365487	0.621857	1.369073
6	1	0	0.891966	1.739941	0.092044
7	7	0	-0.956466	0.903257	-0.270084
8	7	0	-1.718504	-0.035026	-0.012733
9	7	0	-2.535061	-0.834540	0.160267
10	7	0	2.570817	-0.486666	0.091737
11	1	0	3.080194	0.378109	-0.064795
12	1	0	2.579405	-0.651891	1.093954

gag, E = -298.1503717 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.186036	-0.369651	0.326659
2	1	0	-1.158861	-0.279892	1.420579
3	1	0	-0.698781	-1.311582	0.056811
4	6	0	-0.403865	0.790628	-0.275534
5	1	0	-0.345375	0.686291	-1.363947
6	1	0	-0.884886	1.740731	-0.039464
7	7	0	0.958320	0.891703	0.302710
8	7	0	1.719784	-0.039905	0.020252
9	7	0	2.534345	-0.837151	-0.170042
10	7	0	-2.538121	-0.376231	-0.235778
11	1	0	-3.020474	-1.224651	0.044088
12	1	0	-3.072514	0.394331	0.155195

gag^{-}, E = -298.1503318 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.205538	-0.305475	-0.393276
2	1	0	1.269345	-0.095697	-1.463953
3	1	0	0.674500	-1.260044	-0.270199
4	6	0	0.402087	0.803218	0.274217
5	1	0	0.354540	0.646322	1.358332
6	1	0	0.862347	1.771344	0.080608
7	7	0	-0.970201	0.894562	-0.279869
8	7	0	-1.714082	-0.055705	-0.013053

9	7	0	-2.516371	-0.867465	0.168055
10	7	0	2.559207	-0.316173	0.164624
11	1	0	2.537598	-0.691955	1.108304
12	1	0	3.146057	-0.942966	-0.377036

aga, E = -298.1520752 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.758876	0.476476	-0.155329
2	1	0	-1.853232	0.680171	-1.226031
3	1	0	-2.441099	1.151363	0.369462
4	6	0	-0.340408	0.810338	0.281344
5	1	0	-0.118667	1.868579	0.103063
6	1	0	-0.209774	0.588928	1.346891
7	7	0	0.583472	-0.031035	-0.523002
8	7	0	1.733978	-0.124018	-0.086832
9	7	0	2.837122	-0.283886	0.216079
10	7	0	-2.174421	-0.901300	0.094551
11	1	0	-1.511545	-1.533056	-0.346423
12	1	0	-2.131036	-1.095198	1.091383

agg, E = -298.1519595 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.744344	0.489779	0.173890
2	1	0	1.827874	0.631554	1.260185
3	1	0	2.410976	1.209032	-0.309903
4	6	0	0.327616	0.812422	-0.248465
5	1	0	0.070662	1.842931	0.017679
6	1	0	0.218198	0.671958	-1.329053
7	7	0	-0.575685	-0.124368	0.472061
8	7	0	-1.745275	-0.140410	0.079069
9	7	0	-2.862198	-0.245998	-0.196023
10	7	0	2.105162	-0.857343	-0.270791
11	1	0	3.063062	-1.059987	-0.000238
12	1	0	1.523438	-1.531866	0.218561

agg^{-}, E = -298.1500388 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.728740	0.495806	-0.161526
2	1	0	-1.772782	0.686202	-1.237251
3	1	0	-2.372420	1.235498	0.334281
4	6	0	-0.313130	0.740879	0.319962
5	1	0	-0.073139	1.807221	0.250949
6	1	0	-0.209226	0.423727	1.364502
7	7	0	0.625027	-0.027633	-0.536022
8	7	0	1.772844	-0.134204	-0.097230
9	7	0	2.875693	-0.304365	0.202934

10	7	0	-2.134279	-0.888741	0.085146
11	1	0	-2.250906	-1.032880	1.084540
12	1	0	-3.045303	-1.055273	-0.331429

gga, E = -298.1521611 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.318153	-0.042831	0.679156
2	1	0	0.708020	-0.686353	1.322003
3	1	0	2.080517	0.416087	1.316294
4	6	0	0.445733	1.073931	0.112805
5	1	0	0.027654	1.686861	0.919929
6	1	0	1.026419	1.713646	-0.553049
7	7	0	-0.653400	0.537330	-0.732477
8	7	0	-1.528642	-0.085054	-0.121236
9	7	0	-2.414112	-0.678099	0.326222
10	7	0	1.981326	-0.879711	-0.317622
11	1	0	1.287659	-1.273178	-0.947384
12	1	0	2.590211	-0.304925	-0.893773

ggg, E = -298.1520207 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.324292	-0.006375	0.660671
2	1	0	0.724766	-0.647524	1.323921
3	1	0	2.096613	0.466976	1.274109
4	6	0	0.436711	1.090093	0.099483
5	1	0	0.014877	1.698099	0.906720
6	1	0	1.005486	1.729637	-0.575041
7	7	0	-0.662184	0.531035	-0.734154
8	7	0	-1.522162	-0.100193	-0.110054
9	7	0	-2.393688	-0.703781	0.350206
10	7	0	1.973074	-0.737378	-0.428774
11	1	0	2.561117	-1.470736	-0.043743
12	1	0	1.265847	-1.206543	-0.987458

ggg^{-}, E = -298.1508925 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.279375	-0.061800	0.638728
2	1	0	0.664679	-0.661312	1.317972
3	1	0	2.120242	0.332694	1.226576
4	6	0	0.479509	1.137225	0.155057
5	1	0	0.181212	1.751899	1.011333
6	1	0	1.073939	1.752777	-0.521651
7	7	0	-0.725872	0.765513	-0.628409
8	7	0	-1.461391	-0.073881	-0.103585
9	7	0	-2.228046	-0.853708	0.271702
10	7	0	1.683716	-0.911639	-0.481005

11	1	0	2.327419	-0.400487	-1.078890
12	1	0	2.200360	-1.712115	-0.128977

g⁻ga, E = -298.1515146 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.686123	-0.129234	-0.120367
2	1	0	1.913813	-0.375549	-1.161016
3	1	0	2.577465	-0.354101	0.474785
4	6	0	0.568648	-1.047698	0.369814
5	1	0	0.869974	-2.091728	0.266614
6	1	0	0.339528	-0.849515	1.423240
7	7	0	-0.661680	-0.901814	-0.448110
8	7	0	-1.456620	-0.031773	-0.078071
9	7	0	-2.298523	0.718587	0.174991
10	7	0	1.414229	1.301991	-0.038771
11	1	0	0.664075	1.562459	-0.670331
12	1	0	1.124682	1.561086	0.899756

g⁻gg, E = -298.1515858 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.671843	-0.124415	-0.098542
2	1	0	1.957765	-0.365052	-1.130478
3	1	0	2.541809	-0.301771	0.540757
4	6	0	0.574926	-1.077721	0.345783
5	1	0	0.881010	-2.112484	0.186196
6	1	0	0.346501	-0.928365	1.406119
7	7	0	-0.656814	-0.896747	-0.464463
8	7	0	-1.439936	-0.026536	-0.070157
9	7	0	-2.272105	0.728853	0.198788
10	7	0	1.235627	1.264335	0.072995
11	1	0	2.044071	1.878033	0.081247
12	1	0	0.680831	1.553122	-0.727424

g⁻gg⁻, E = -298.1523262 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.619902	-0.116340	-0.210454
2	1	0	1.688531	-0.280182	-1.288971
3	1	0	2.594433	-0.367290	0.232473
4	6	0	0.590597	-1.076832	0.362626
5	1	0	0.922816	-2.106826	0.229857
6	1	0	0.447260	-0.894042	1.434557
7	7	0	-0.709257	-0.990683	-0.340162
8	7	0	-1.423409	-0.019871	-0.071091
9	7	0	-2.217224	0.802513	0.098974
10	7	0	1.201528	1.266443	0.021853
11	1	0	1.318062	1.497884	1.004744

12	1	0	1.804441	1.900669	-0.492709

2-Azidoethylammonium ion

aa, E = -298.5975656 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.479848	0.533672	-0.048601
2	1	0	1.544728	1.231815	0.784550
3	1	0	1.482745	1.079954	-0.990256
4	6	0	0.247909	-0.345555	0.069243
5	1	0	0.184702	-1.032722	-0.781449
6	1	0	0.270736	-0.923294	0.999784
7	7	0	-0.893123	0.588367	0.072141
8	7	0	-2.004695	0.048445	-0.001588
9	7	0	-3.094369	-0.321278	-0.064691
10	7	0	2.715423	-0.306920	-0.019556
11	1	0	2.808903	-0.817765	0.861501
12	1	0	2.724196	-0.995014	-0.776295
13	1	0	3.554788	0.268029	-0.125834

ag, E = -298.5974339 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.149794	-0.311983	-0.404076
2	1	0	1.232310	-0.094664	-1.467893
3	1	0	0.728216	-1.307002	-0.264482
4	6	0	0.320748	0.753817	0.303659
5	1	0	0.229744	0.535486	1.372957
6	1	0	0.775781	1.736942	0.181526
7	7	0	-1.005702	0.847832	-0.329882
8	7	0	-1.804310	-0.048914	-0.018082
9	7	0	-2.652876	-0.801610	0.187402
10	7	0	2.539811	-0.346655	0.149948
11	1	0	3.026102	0.542630	0.009061
12	1	0	2.547288	-0.548129	1.153023
13	1	0	3.098839	-1.070845	-0.307391

ga, E = -298.6022925 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.682447	0.582742	-0.197037
2	1	0	-1.780118	0.684960	-1.276811
3	1	0	-2.388976	1.242682	0.303676
4	6	0	-0.265093	0.856834	0.253787
5	1	0	0.013732	1.867751	-0.057187
6	1	0	-0.178980	0.779533	1.343070
7	7	0	0.580610	-0.158750	-0.409441
8	7	0	1.772032	-0.152655	-0.073603

9	7	0	2.897711	-0.245746	0.152062
10	7	0	-2.048405	-0.826146	0.141713
11	1	0	-1.350456	-1.469781	-0.244273
12	1	0	-2.080632	-0.977323	1.152610
13	1	0	-2.962959	-1.082206	-0.236699

gg, E = -298.6013585 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.302012	0.156151	0.718296
2	1	0	0.779983	-0.470499	1.441148
3	1	0	2.090218	0.714400	1.222530
4	6	0	0.347045	1.087752	-0.008123
5	1	0	-0.127701	1.750106	0.720935
6	1	0	0.877898	1.698112	-0.739431
7	7	0	-0.653529	0.316343	-0.777649
8	7	0	-1.598258	-0.130981	-0.108062
9	7	0	-2.533896	-0.589804	0.384233
10	7	0	1.951612	-0.763722	-0.265484
11	1	0	1.241986	-1.241129	-0.829633
12	1	0	2.566259	-0.259188	-0.908434
13	1	0	2.515512	-1.478070	0.200584

2-Azidoethanol

aaa, E = -318.0015734 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.583464	0.475397	-0.081927
2	1	0	-1.556130	0.977282	-1.054349
3	1	0	-1.629015	1.233343	0.707635
4	6	0	-0.332902	-0.360837	0.095709
5	1	0	-0.389854	-0.922959	1.033426
6	1	0	-0.223901	-1.060279	-0.738974
7	7	0	0.811143	0.578585	0.138776
8	7	0	1.923573	0.061670	-0.000101
9	7	0	3.015360	-0.296284	-0.112786
10	1	0	-3.475586	0.067387	-0.237789
11	8	0	-2.684731	-0.423741	0.003267

aag, E = -318.001886 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.592887	0.492077	-0.051282
2	1	0	-1.567721	1.073514	-0.973813
3	1	0	-1.644685	1.182608	0.797229
4	6	0	-0.335552	-0.354958	0.055909
5	1	0	-0.366419	-0.972568	0.960611
6	1	0	-0.248638	-1.005837	-0.819864

7	7	0	0.812204	0.579481	0.127270
8	7	0	1.924066	0.056722	0.005468
9	7	0	3.015404	-0.307290	-0.091916
10	1	0	-2.844333	-0.778329	0.720791
11	8	0	-2.752411	-0.328061	-0.124808

gaa, E = -318.0019064 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.221853	-0.345576	0.360241
2	1	0	-1.289850	-0.176060	1.439805
3	1	0	-0.722178	-1.305804	0.184385
4	6	0	-0.420663	0.779266	-0.273661
5	1	0	-0.349272	0.634281	-1.356581
6	1	0	-0.896296	1.738721	-0.073862
7	7	0	0.929507	0.868341	0.325965
8	7	0	1.707310	-0.043332	0.019725
9	7	0	2.538838	-0.816993	-0.189665
10	1	0	-3.055114	-0.967870	0.206172
11	8	0	-2.507722	-0.322690	-0.251447

gag, E = -318.0021934 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.224570	-0.336433	-0.390675
2	1	0	1.287214	-0.129588	-1.459974
3	1	0	0.724336	-1.302147	-0.251881
4	6	0	0.427428	0.769171	0.293139
5	1	0	0.362555	0.589485	1.372473
6	1	0	0.906292	1.733155	0.124990
7	7	0	-0.929078	0.884914	-0.288410
8	7	0	-1.705952	-0.038273	-0.015937
9	7	0	-2.537885	-0.818406	0.167158
10	1	0	2.527186	-0.652153	1.015366
11	8	0	2.561355	-0.379103	0.093071

gag^{-}, E = -318.0021896 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.214565	-0.369863	0.357938
2	1	0	-1.259795	-0.212061	1.440644
3	1	0	-0.718620	-1.324230	0.167442
4	6	0	-0.428243	0.765037	-0.289729
5	1	0	-0.360316	0.609850	-1.371382
6	1	0	-0.913159	1.723511	-0.101207
7	7	0	0.922620	0.883075	0.305414
8	7	0	1.708049	-0.028953	0.020530
9	7	0	2.545650	-0.800703	-0.171968
10	1	0	-3.007435	0.306570	0.043201

11	8	0	-2.514758	-0.481077	-0.208224

aga, E = -318.0032008 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.737259	0.464462	0.192121
2	1	0	1.779406	0.546568	1.283386
3	1	0	2.397744	1.221403	-0.245713
4	6	0	0.330455	0.737249	-0.277527
5	1	0	0.079830	1.787234	-0.092572
6	1	0	0.251511	0.530592	-1.350260
7	7	0	-0.595570	-0.138658	0.480622
8	7	0	-1.764426	-0.137503	0.084812
9	7	0	-2.883807	-0.224552	-0.186433
10	1	0	2.953053	-1.050127	0.165870
11	8	0	2.104849	-0.842618	-0.237660

agg, E = -318.003035 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.751667	0.456984	-0.166871
2	1	0	-1.821342	0.623548	-1.243161
3	1	0	-2.427756	1.155997	0.338520
4	6	0	-0.339863	0.743089	0.300219
5	1	0	-0.122557	1.809592	0.171760
6	1	0	-0.229821	0.486140	1.360283
7	7	0	0.597086	-0.062221	-0.517528
8	7	0	1.753108	-0.123990	-0.089915
9	7	0	2.862495	-0.258028	0.201893
10	1	0	-2.145225	-1.041417	1.001897
11	8	0	-2.149118	-0.890578	0.051182

agg^{-}, E = -318.0050563 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.773073	0.426201	0.146323
2	1	0	1.898276	0.574407	1.224958
3	1	0	2.489876	1.057845	-0.380867
4	6	0	0.369518	0.823198	-0.257215
5	1	0	0.186211	1.876913	-0.022484
6	1	0	0.226207	0.652085	-1.328872
7	7	0	-0.556810	-0.037083	0.522661
8	7	0	-1.709076	-0.112569	0.085079
9	7	0	-2.812750	-0.258753	-0.219437
10	1	0	1.385286	-1.460999	0.198702
11	8	0	2.063631	-0.917226	-0.218025

gga, E = -318.0032189 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.309438	-0.112546	0.630142
2	1	0	0.694149	-0.838034	1.175976
3	1	0	2.081264	0.265158	1.311252
4	6	0	0.459289	1.058412	0.185967
5	1	0	0.093616	1.600683	1.064729
6	1	0	1.048478	1.738389	-0.428870
7	7	0	-0.682746	0.649408	-0.667472
8	7	0	-1.516271	-0.076487	-0.116235
9	7	0	-2.365939	-0.754912	0.275021
10	1	0	2.314470	-1.522196	-0.247930
11	8	0	1.888794	-0.705658	-0.526377

ggg, E = -318.003423 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.303787	-0.125881	0.635960
2	1	0	0.687345	-0.787039	1.249823
3	1	0	2.133264	0.236223	1.254917
4	6	0	0.493998	1.076636	0.180072
5	1	0	0.165431	1.647524	1.056377
6	1	0	1.095235	1.729041	-0.454221
7	7	0	-0.675128	0.703646	-0.650986
8	7	0	-1.486507	-0.056171	-0.112872
9	7	0	-2.320247	-0.759287	0.269156
10	1	0	2.342292	-0.368674	-0.985717
11	8	0	1.770363	-0.922364	-0.444307

***ggg*⁻**, E = -318.004656 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.348429	-0.054535	0.658535
2	1	0	0.755796	-0.717189	1.301889
3	1	0	2.141525	0.391208	1.262296
4	6	0	0.467505	1.048761	0.101176
5	1	0	0.050289	1.655233	0.912471
6	1	0	1.043303	1.686473	-0.568898
7	7	0	-0.622828	0.486851	-0.738376
8	7	0	-1.525418	-0.081822	-0.111405
9	7	0	-2.435223	-0.624159	0.349095
10	1	0	1.292172	-1.115663	-0.957647
11	8	0	1.988200	-0.791439	-0.375447

g⁻ga, E = -318.0051413 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.609075	-0.020125	-0.201281

2	1	0	1.699090	-0.141157	-1.285814
3	1	0	2.592124	-0.169347	0.260591
4	6	0	0.652912	-1.056826	0.345402
5	1	0	1.048674	-2.056343	0.165799
6	1	0	0.518679	-0.916178	1.423537
7	7	0	-0.657320	-1.017930	-0.340725
8	7	0	-1.388390	-0.059729	-0.066330
9	7	0	-2.189338	0.754797	0.104332
10	1	0	1.621974	1.923285	-0.306104
11	8	0	1.074109	1.260186	0.124542

g⁻gg, E = -318.0049439 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.602330	-0.010066	-0.231533
2	1	0	1.664918	-0.149653	-1.311870
3	1	0	2.600275	-0.143304	0.201862
4	6	0	0.662613	-1.045997	0.360046
5	1	0	1.064503	-2.047405	0.200918
6	1	0	0.539562	-0.884655	1.437536
7	7	0	-0.657027	-1.034980	-0.306601
8	7	0	-1.386596	-0.067715	-0.061656
9	7	0	-2.188856	0.749975	0.088711
10	1	0	1.206946	1.514281	0.906632
11	8	0	1.120187	1.314518	-0.031168

g⁻gg⁻, E = -318.0051412 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.609083	-0.020271	-0.201602
2	1	0	1.698329	-0.141214	-1.286249
3	1	0	2.592423	-0.169760	0.259517
4	6	0	0.652870	-1.056719	0.345493
5	1	0	1.048361	-2.056308	0.165793
6	1	0	0.518860	-0.916019	1.423645
7	7	0	-0.657422	-1.017860	-0.340504
8	7	0	-1.388558	-0.059594	-0.066296
9	7	0	-2.189665	0.754855	0.104116
10	1	0	1.621930	1.923071	-0.306683
11	8	0	1.074737	1.260045	0.124927

Protonated 2-azidoethanol

aaa, E = -318.3939478 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.461508	0.535300	0.101344
2	1	0	-1.572454	1.285331	-0.676855

3	1	0	-1.476918	0.989578	1.088005
4	6	0	-0.262334	-0.363998	-0.121930
5	1	0	-0.167059	-1.091747	0.689240
6	1	0	-0.344251	-0.886620	-1.079930
7	7	0	0.873659	0.574217	-0.138397
8	7	0	1.984965	0.045478	0.000259
9	7	0	3.073234	-0.312889	0.115759
10	1	0	-2.895095	-0.680573	-0.814334
11	1	0	-2.847060	-0.887504	0.758015
12	8	0	-2.734640	-0.237990	0.039504

aag, E = -318.3943164 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.456132	0.530579	0.083295
2	1	0	-1.572214	1.248670	-0.724829
3	1	0	-1.467507	1.012513	1.056365
4	6	0	-0.259652	-0.377451	-0.098126
5	1	0	-0.153702	-1.037376	0.766872
6	1	0	-0.359257	-0.976342	-1.008880
7	7	0	0.874883	0.555054	-0.215949
8	7	0	1.985775	0.049824	-0.005985
9	7	0	3.073660	-0.288882	0.161051
10	1	0	-3.448307	0.084072	0.483750
11	1	0	-2.912566	-0.681921	-0.791179
12	8	0	-2.666495	-0.347544	0.091633

gaa, E = -318.394104 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.171202	-0.267550	-0.453693
2	1	0	1.333510	0.073350	-1.472341
3	1	0	0.788062	-1.285092	-0.439635
4	6	0	0.331467	0.703087	0.360906
5	1	0	0.217795	0.361112	1.393634
6	1	0	0.774555	1.698331	0.356457
7	7	0	-0.970456	0.830220	-0.316083
8	7	0	-1.805689	-0.040805	-0.021324
9	7	0	-2.684806	-0.760430	0.167916
10	1	0	3.085635	0.405524	0.077703
11	1	0	2.587601	-0.781722	1.004180
12	8	0	2.552935	-0.410951	0.102895

gag, E = -318.3943798 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.153313	-0.274315	0.432601
2	1	0	-1.321081	-0.002838	1.472031
3	1	0	-0.752186	-1.280510	0.340422

4	6	0	-0.329773	0.750312	-0.326012
5	1	0	-0.240062	0.470435	-1.378868
6	1	0	-0.771694	1.743262	-0.248960
7	7	0	0.984595	0.839082	0.333527
8	7	0	1.792006	-0.051094	0.018779
9	7	0	2.647409	-0.794586	-0.187459
10	1	0	-2.970045	-1.188755	-0.019883
11	1	0	-3.080866	0.385858	-0.046621
12	8	0	-2.491704	-0.367156	-0.238947

***gag*⁻**, E = -318.3945412 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.175141	-0.266742	-0.441810
2	1	0	1.343334	0.076921	-1.458719
3	1	0	0.807438	-1.290578	-0.420514
4	6	0	0.324809	0.708818	0.351049
5	1	0	0.209654	0.386262	1.389864
6	1	0	0.775700	1.699686	0.326796
7	7	0	-0.976432	0.820830	-0.328851
8	7	0	-1.809149	-0.049087	-0.025052
9	7	0	-2.686209	-0.769713	0.170283
10	1	0	2.598360	-0.792003	1.000168
11	1	0	3.235435	-0.585476	-0.430567
12	8	0	2.541614	-0.270185	0.177860

aga, E = -318.4006663 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.734892	0.533272	-0.149016
2	1	0	-1.924797	0.650460	-1.212147
3	1	0	-2.504048	1.011302	0.450436
4	6	0	-0.326408	0.917620	0.238056
5	1	0	-0.122129	1.927406	-0.128335
6	1	0	-0.188616	0.881517	1.322346
7	7	0	0.517666	-0.093524	-0.435932
8	7	0	1.703987	-0.122789	-0.072810
9	7	0	2.821613	-0.234659	0.171269
10	1	0	-1.006514	-1.344685	-0.142339
11	1	0	-2.125190	-1.177071	0.983064
12	8	0	-1.882971	-0.937185	0.069380

agg, E = -318.4015986 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.728374	0.541356	-0.160621
2	1	0	-1.905435	0.596355	-1.232507
3	1	0	-2.483731	1.068878	0.413880
4	6	0	-0.318665	0.914969	0.220606

5	1	0	-0.100929	1.914867	-0.163823
6	1	0	-0.194860	0.896874	1.306908
7	7	0	0.520300	-0.119133	-0.424969
8	7	0	1.710633	-0.130899	-0.074645
9	7	0	2.831156	-0.232920	0.160908
10	1	0	-2.635105	-1.339409	-0.132465
11	1	0	-1.029553	-1.349888	-0.069132
12	8	0	-1.850347	-0.893121	0.236021

***agg*⁻**, E = -318.397889 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.658587	0.584551	-0.197655
2	1	0	-1.731911	0.646493	-1.280009
3	1	0	-2.364004	1.246834	0.298848
4	6	0	-0.255054	0.771906	0.299541
5	1	0	-0.002930	1.824562	0.126894
6	1	0	-0.190504	0.575801	1.375563
7	7	0	0.623989	-0.124006	-0.468720
8	7	0	1.801357	-0.146760	-0.085349
9	7	0	2.919121	-0.264037	0.167301
10	1	0	-2.102119	-1.026659	1.054395
11	1	0	-2.943077	-1.054399	-0.281201
12	8	0	-2.074359	-0.825969	0.100196

gga, E = -318.399517 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.432531	0.399611	0.620991
2	1	0	1.037865	0.095868	1.587222
3	1	0	2.336249	0.993842	0.728405
4	6	0	0.384053	1.013997	-0.285963
5	1	0	-0.122372	1.827827	0.238090
6	1	0	0.834192	1.397029	-1.201466
7	7	0	-0.537260	-0.073091	-0.694147
8	7	0	-1.603604	-0.143161	-0.056895
9	7	0	-2.630650	-0.299995	0.434638
10	1	0	1.046476	-1.264152	-0.442305
11	1	0	2.551944	-0.788953	-0.675416
12	8	0	1.852092	-0.891173	-0.003734

ggg, E = -318.400367 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.437753	0.392579	0.615119
2	1	0	1.053011	0.031798	1.567371
3	1	0	2.323755	1.009848	0.735022
4	6	0	0.374029	1.022172	-0.259290
5	1	0	-0.130338	1.815638	0.296351

6	1	0	0.817899	1.436020	-1.164346
7	7	0	-0.546709	-0.054808	-0.693826
8	7	0	-1.607222	-0.148261	-0.050746
9	7	0	-2.629949	-0.325029	0.443422
10	1	0	2.419323	-1.431826	0.350382
11	1	0	1.068945	-1.247078	-0.502208
12	8	0	1.882985	-0.800779	-0.163686

ggg⁻, E = -318.39718 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.264833	0.027951	0.727175
2	1	0	0.735731	-0.748730	1.274621
3	1	0	2.051500	0.476286	1.331026
4	6	0	0.350240	1.061454	0.116969
5	1	0	-0.076879	1.636210	0.946389
6	1	0	0.909040	1.750862	-0.516100
7	7	0	-0.691759	0.470681	-0.736612
8	7	0	-1.602024	-0.111693	-0.127477
9	7	0	-2.512156	-0.674355	0.300811
10	1	0	2.523638	-0.169160	-0.927718
11	1	0	2.421860	-1.502744	-0.087783
12	8	0	1.923280	-0.721448	-0.392795

g⁻gg⁻, E = -318.3975246 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.621754	-0.230707	-0.180487
2	1	0	1.716306	-0.328539	-1.258325
3	1	0	2.573402	-0.371260	0.328531
4	6	0	0.518842	-1.093328	0.378719
5	1	0	0.848945	-2.128265	0.275203
6	1	0	0.357635	-0.893172	1.442815
7	7	0	-0.725528	-0.965686	-0.394830
8	7	0	-1.460625	-0.019643	-0.073059
9	7	0	-2.248345	0.797957	0.125280
10	1	0	1.342501	1.527928	0.923122
11	1	0	1.662322	1.818134	-0.597216
12	8	0	1.212100	1.203874	0.011843

N-(2-Azidoethyl)ethanamide

aag, E = -450.5141786 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.124893	0.911049	-0.574480
2	1	0	-0.164693	1.958261	-0.676899
3	1	0	0.199490	0.466069	-1.569187
4	6	0	-0.915061	0.156692	0.242375

5	1	0	-0.603164	-0.883904	0.372875
6	1	0	-1.037248	0.627246	1.223665
7	7	0	-2.187405	0.212614	-0.517214
8	7	0	-3.181984	-0.187045	0.096162
9	7	0	-4.182414	-0.531995	0.558248
10	7	0	1.424600	0.853876	0.062822
11	1	0	1.711508	1.613713	0.661465
12	6	0	2.229973	-0.233141	-0.053447
13	6	0	3.539999	-0.167647	0.694990
14	1	0	3.686922	0.779036	1.216647
15	1	0	3.567774	-0.985183	1.418618
16	1	0	4.354407	-0.318208	-0.016447
17	8	0	1.912076	-1.211361	-0.735936

gag, E = -450.51487 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.102376	-0.747779	-0.684563
2	1	0	0.361589	-1.574513	-1.348260
3	1	0	0.352377	0.192857	-1.182799
4	6	0	0.879627	-0.864718	0.626652
5	1	0	0.577164	-0.070014	1.315661
6	1	0	0.694301	-1.832225	1.092664
7	7	0	2.340473	-0.809518	0.387411
8	7	0	2.770276	0.296246	0.036580
9	7	0	3.304647	1.268943	-0.284000
10	7	0	-1.326243	-0.772512	-0.446272
11	1	0	-1.821596	-1.648955	-0.516376
12	6	0	-1.992834	0.333716	-0.025997
13	6	0	-3.470666	0.159505	0.229212
14	1	0	-3.821193	-0.854626	0.033168
15	1	0	-3.676008	0.416614	1.270503
16	1	0	-4.017566	0.859462	-0.405837
17	8	0	-1.423019	1.418118	0.126677

***gag*$^{-}$**, E = -450.5145153 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.160975	-0.350492	-0.513613
2	1	0	-0.079972	0.331770	-1.362502
3	1	0	-0.732493	-1.228570	-0.823597
4	6	0	-0.859832	0.362648	0.643815
5	1	0	-0.963957	-0.310718	1.501438
6	1	0	-0.283006	1.236577	0.942795
7	7	0	-2.184855	0.880285	0.232275
8	7	0	-3.047064	0.018270	0.023856
9	7	0	-3.946146	-0.674261	-0.192195
10	7	0	1.166675	-0.785903	-0.131255
11	1	0	1.294717	-1.724974	0.215175
12	6	0	2.218155	0.073656	-0.108386
13	6	0	3.533882	-0.504572	0.355232

14	1	0	3.466835	-1.560686	0.619978
15	1	0	4.268412	-0.379231	-0.443025
16	1	0	3.876922	0.063486	1.222466
17	8	0	2.105612	1.252022	-0.457973

agg, E = -450.5160516 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.228551	-1.448376	-0.446474
2	1	0	-0.084690	-1.928868	-1.375426
3	1	0	0.773459	-2.176724	0.157844
4	6	0	-0.986586	-0.978965	0.334606
5	1	0	-1.635717	-1.830327	0.566731
6	1	0	-0.670688	-0.496699	1.264906
7	7	0	-1.709218	-0.005359	-0.520192
8	7	0	-2.697555	0.520023	0.001059
9	7	0	-3.636589	1.079833	0.373569
10	7	0	1.121953	-0.356450	-0.776937
11	1	0	0.964449	0.149666	-1.635641
12	6	0	1.961714	0.179481	0.145553
13	6	0	2.726275	1.405639	-0.293561
14	1	0	2.605020	1.624855	-1.355365
15	1	0	2.374364	2.259770	0.290245
16	1	0	3.784518	1.257183	-0.071530
17	8	0	2.094927	-0.308982	1.271875

***agg*$^-$**, E = -450.5151933 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.223859	1.560293	0.175146
2	1	0	0.355142	1.439018	1.250852
3	1	0	0.397929	2.608747	-0.083283
4	6	0	-1.194807	1.191135	-0.221098
5	1	0	-1.903174	1.842860	0.302252
6	1	0	-1.334166	1.306187	-1.302022
7	7	0	-1.418506	-0.223331	0.161031
8	7	0	-2.571627	-0.631872	-0.004177
9	7	0	-3.607226	-1.131048	-0.116934
10	7	0	1.205932	0.724913	-0.482973
11	1	0	1.326097	0.821655	-1.481069
12	6	0	1.897456	-0.256287	0.153420
13	6	0	2.806804	-1.081586	-0.727725
14	1	0	2.883708	-0.695535	-1.745173
15	1	0	3.799492	-1.112528	-0.275053
16	1	0	2.418651	-2.102484	-0.761696
17	8	0	1.799555	-0.469986	1.364763

ggg, E = -450.5159593 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.145763	0.730201	0.922592
2	1	0	-0.834130	0.377515	1.694781
3	1	0	0.384841	1.603302	1.311528
4	6	0	-0.911708	1.148747	-0.327911
5	1	0	-1.593283	1.973457	-0.091618
6	1	0	-0.218646	1.469364	-1.103733
7	7	0	-1.665805	0.016689	-0.918715
8	7	0	-2.608023	-0.403930	-0.238225
9	7	0	-3.514316	-0.888005	0.290797
10	7	0	0.812314	-0.324464	0.658847
11	1	0	0.543324	-1.283076	0.821828
12	6	0	1.987436	-0.073470	0.028146
13	6	0	2.848208	-1.277955	-0.269860
14	1	0	2.451311	-2.200661	0.155627
15	1	0	2.926227	-1.388154	-1.354070
16	1	0	3.849935	-1.097869	0.124674
17	8	0	2.331524	1.072369	-0.278219

***ggg*⁻**, E = -450.5170655 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.138523	1.371789	-0.773783
2	1	0	0.382432	0.637548	-1.544495
3	1	0	0.017399	2.346724	-1.254085
4	6	0	1.269096	1.464419	0.246539
5	1	0	2.191508	1.787880	-0.249347
6	1	0	1.018975	2.181468	1.028693
7	7	0	1.487872	0.181187	0.952651
8	7	0	1.937491	-0.733324	0.253508
9	7	0	2.361920	-1.666470	-0.278369
10	7	0	-1.116519	0.977371	-0.169988
11	1	0	-1.645918	1.669979	0.339307
12	6	0	-1.544975	-0.311709	-0.147124
13	6	0	-2.827286	-0.558773	0.612622
14	1	0	-3.326582	0.361426	0.919437
15	1	0	-3.499416	-1.145392	-0.016033
16	1	0	-2.592731	-1.150059	1.501249
17	8	0	-0.931644	-1.224409	-0.707358

g*⁻*gg, E = -450.5176513 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.298124	-1.565057	0.588672
2	1	0	0.753905	-1.833553	1.543030
3	1	0	-0.250085	-2.429948	0.203042
4	6	0	1.385359	-1.188448	-0.413119
5	1	0	2.087282	-2.015119	-0.525896
6	1	0	0.945405	-0.956216	-1.386953
7	7	0	2.188101	-0.039968	0.068688
8	7	0	1.670241	1.073070	-0.079339

9	7	0	1.327867	2.172310	-0.184170
10	7	0	-0.623482	-0.471364	0.829740
11	1	0	-0.570427	0.032367	1.702560
12	6	0	-1.558968	-0.104381	-0.084026
13	6	0	-2.392096	1.100693	0.280147
14	1	0	-2.368678	1.323000	1.348091
15	1	0	-2.003776	1.964642	-0.266882
16	1	0	-3.421373	0.929612	-0.037133
17	8	0	-1.688232	-0.701245	-1.156792

g⁻gg⁻, E = -450.5175991 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.640040	-1.629472	-0.050887
2	1	0	0.483085	-1.763071	1.020145
3	1	0	0.734939	-2.612897	-0.520794
4	6	0	1.923317	-0.840830	-0.288399
5	1	0	2.777138	-1.401801	0.092808
6	1	0	2.071251	-0.655404	-1.358266
7	7	0	1.930517	0.440196	0.451077
8	7	0	1.176951	1.324171	0.028311
9	7	0	0.557709	2.257613	-0.259943
10	7	0	-0.522280	-0.948112	-0.583995
11	1	0	-0.677769	-0.971726	-1.581797
12	6	0	-1.425797	-0.289629	0.191997
13	6	0	-2.531133	0.408943	-0.562475
14	1	0	-2.649957	0.038564	-1.581983
15	1	0	-3.466611	0.287198	-0.015220
16	1	0	-2.291955	1.475673	-0.600982
17	8	0	-1.327371	-0.225959	1.419565

Water
1,2-Diazidoethane

aaa, E = -406.1999089 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.397121	0.645393	0.118890
2	1	0	-1.059017	0.678602	0.990282
3	1	0	-0.995640	0.722063	-0.794091
4	6	0	0.397121	-0.645393	0.118890
5	1	0	0.995640	-0.722063	-0.794091
6	1	0	1.059017	-0.678602	0.990282
7	7	0	0.591307	1.743853	0.189287
8	7	0	0.144880	2.869280	-0.056955
9	7	0	-0.144880	3.967264	-0.262265
10	7	0	-0.591307	-1.743853	0.189287
11	7	0	-0.144880	-2.869280	-0.056955
12	7	0	0.144880	-3.967264	-0.262265

aag, E = -406.2002744 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.398848	0.003382	0.227167
2	1	0	-0.536271	0.041933	1.312529
3	1	0	-0.103757	-1.011073	-0.064001
4	6	0	0.657679	1.011987	-0.195947
5	1	0	0.776142	1.006315	-1.284415
6	1	0	0.373799	2.012861	0.126716
7	7	0	-1.647164	0.382107	-0.473157
8	7	0	-2.666885	-0.185118	-0.065951
9	7	0	-3.686900	-0.644196	0.217824
10	7	0	1.944917	0.724562	0.470702
11	7	0	2.545181	-0.274554	0.053532
12	7	0	3.216152	-1.165980	-0.242685

gag, E = -406.2007694 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.750604	0.139557	-0.702255
2	1	0	-1.028430	0.685986	-1.602842
3	1	0	-1.037450	0.730050	0.175198
4	6	0	0.750604	-0.139557	-0.702255
5	1	0	1.037450	-0.730050	0.175198
6	1	0	1.028430	-0.685986	-1.602842
7	7	0	-1.517061	-1.124397	-0.740989
8	7	0	-1.517061	-1.771052	0.314991
9	7	0	-1.613391	-2.465860	1.231880
10	7	0	1.517061	1.124397	-0.740989
11	7	0	1.517061	1.771052	0.314991
12	7	0	1.613391	2.465860	1.231880

gag^{-}, E = -406.2006375 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.365910	-0.615090	0.265236
2	1	0	0.365964	-0.621745	1.355736
3	1	0	1.401231	-0.622643	-0.090519
4	6	0	-0.365910	0.615090	-0.265236
5	1	0	-0.365964	0.621745	-1.355736
6	1	0	-1.401231	0.622643	0.090519
7	7	0	-0.336012	-1.853402	-0.135298
8	7	0	-0.247845	-2.144097	-1.335520
9	7	0	-0.238252	-2.540409	-2.419742
10	7	0	0.336012	1.853402	0.135298
11	7	0	0.247845	2.144097	1.335520
12	7	0	0.238252	2.540409	2.419742

aga, E = -406.2021528 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.320853	-0.682679	0.977608
2	1	0	-0.041140	-1.209944	1.895714
3	1	0	-1.410752	-0.586608	0.932539
4	6	0	0.320853	0.682679	0.977608
5	1	0	0.041140	1.209944	1.895714
6	1	0	1.410752	0.586608	0.932539
7	7	0	-0.179402	1.419396	-0.204725
8	7	0	0.320853	2.535148	-0.379874
9	7	0	0.179402	-1.419396	-0.204725
10	7	0	-0.320853	-2.535148	-0.379874
11	7	0	0.710098	3.586128	-0.657387
12	7	0	-0.710098	-3.586128	-0.657387

agg, E = -406.2022324 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.886237	1.388619	0.083333
2	1	0	-1.529370	1.757980	0.889295
3	1	0	-0.666340	2.209258	-0.598850
4	6	0	0.395724	0.841775	0.678764
5	1	0	0.869567	1.619599	1.287393
6	1	0	0.186228	-0.023542	1.318455
7	7	0	1.287421	0.455587	-0.436546
8	7	0	2.205847	-0.314037	-0.135649
9	7	0	-1.608403	0.385306	-0.730395
10	7	0	-1.994806	-0.614289	-0.113449
11	7	0	3.103055	-1.024490	0.013911
12	7	0	-2.409830	-1.594599	0.335146

***agg*$^{-}$**, E = -406.2035915 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.000897	1.396086	0.263774
2	1	0	1.362552	2.385424	-0.016514
3	1	0	1.145573	1.255860	1.340076
4	6	0	-0.467602	1.282928	-0.089631
5	1	0	-1.029145	2.068402	0.428504
6	1	0	-0.603711	1.386426	-1.170932
7	7	0	-0.923592	-0.053369	0.356794
8	7	0	-2.076737	-0.355565	0.034435
9	7	0	1.827522	0.436632	-0.497907
10	7	0	1.808337	-0.733683	-0.096178
11	7	0	-3.134164	-0.752774	-0.202945
12	7	0	1.916485	-1.851269	0.173515

ggg, E = -406.2023662 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.709889	-0.275252	1.032187
2	1	0	-0.852036	-0.897155	1.923097
3	1	0	-1.442547	0.532352	1.054227
4	6	0	0.709889	0.275252	1.032187
5	1	0	0.852036	0.897155	1.923097
6	1	0	1.442547	-0.532352	1.054227
7	7	0	1.020449	1.043799	-0.192430
8	7	0	0.297620	2.025200	-0.400881
9	7	0	-1.020449	-1.043799	-0.192430
10	7	0	-0.297620	-2.025200	-0.400881
11	7	0	-0.297620	2.963331	-0.716752
12	7	0	0.297620	-2.963331	-0.716752

g⁻gg⁻, E = -406.2037031 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.260727	-0.715625	1.557914
2	1	0	0.102096	-1.226331	2.451121
3	1	0	-1.354910	-0.721764	1.560374
4	6	0	0.260727	0.715625	1.557914
5	1	0	-0.102096	1.226331	2.451121
6	1	0	1.354910	0.721764	1.560374
7	7	0	-0.260727	1.483727	0.407237
8	7	0	0.391858	1.396695	-0.640741
9	7	0	0.260727	-1.483727	0.407237
10	7	0	-0.391858	-1.396695	-0.640741
11	7	0	0.905786	1.427204	-1.674921
12	7	0	-0.905786	-1.427204	-1.674921

ggg⁻, E = -406.2038339 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.445882	1.490467	-0.381798
2	1	0	-1.230335	2.133003	0.033523
3	1	0	-0.019811	1.966741	-1.263978
4	6	0	0.637579	1.262908	0.662840
5	1	0	1.048760	2.224922	0.970555
6	1	0	0.230377	0.760246	1.548096
7	7	0	1.773879	0.493827	0.115726
8	7	0	1.577878	-0.718047	-0.041311
9	7	0	-1.019179	0.213889	-0.865114
10	7	0	-1.699266	-0.409764	-0.040721
11	7	0	1.555628	-1.860183	-0.213371
12	7	0	-2.357393	-1.091888	0.619871

2-Azidoethanamine

aaa, E = -298.1506449 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.497066	0.746759	0.000000
2	1	0	-1.945580	0.283183	0.882839
3	1	0	-1.945580	0.283183	-0.882839
4	6	0	0.000000	0.463305	0.000000
5	1	0	0.468091	0.894907	-0.892218
6	1	0	0.468091	0.894907	0.892218
7	7	0	0.181981	-1.011123	0.000000
8	7	0	1.354086	-1.397745	0.000000
9	7	0	2.402280	-1.883610	0.000000
10	7	0	-1.826527	2.169437	0.000000
11	1	0	-1.422686	2.622362	0.814525
12	1	0	-1.422686	2.622362	-0.814525

aag, E = -298.1500906 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.579592	0.494308	-0.043961
2	1	0	1.585686	1.181991	0.811933
3	1	0	1.563795	1.094285	-0.957155
4	6	0	0.317375	-0.346689	0.018001
5	1	0	0.223726	-0.952769	-0.888735
6	1	0	0.345052	-1.010901	0.889659
7	7	0	-0.836014	0.579449	0.139411
8	7	0	-1.946343	0.056179	0.010187
9	7	0	-3.037013	-0.311044	-0.089230
10	7	0	2.739727	-0.397717	-0.093625
11	1	0	3.578040	0.142479	-0.282722
12	1	0	2.879401	-0.828864	0.815579

gaa, E = -298.1511552 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.196874	-0.352054	-0.384701
2	1	0	1.212760	-0.176285	-1.463738
3	1	0	0.678328	-1.300797	-0.213518
4	6	0	0.414441	0.778375	0.285091
5	1	0	0.365455	0.621520	1.369052
6	1	0	0.892085	1.739756	0.092172
7	7	0	-0.956374	0.903086	-0.270192
8	7	0	-1.718621	-0.034952	-0.012748
9	7	0	-2.535333	-0.834287	0.160340
10	7	0	2.570954	-0.486577	0.091762
11	1	0	3.079885	0.378538	-0.064493
12	1	0	2.579215	-0.651546	1.094045

gag, E = -298.1504917 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.185963	-0.369726	0.326472
2	1	0	-1.158865	-0.280149	1.420389
3	1	0	-0.698679	-1.311576	0.056420
4	6	0	-0.403916	0.790727	-0.275506
5	1	0	-0.345257	0.686651	-1.363934
6	1	0	-0.884943	1.740751	-0.039170
7	7	0	0.958343	0.891689	0.302743
8	7	0	1.719782	-0.039904	0.020287
9	7	0	2.534308	-0.837172	-0.170045
10	7	0	-2.538175	-0.376268	-0.235791
11	1	0	-3.020483	-1.224507	0.044784
12	1	0	-3.072303	0.394414	0.155358

***gag*⁻**, E = -298.1504552 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.205606	-0.305402	-0.393353
2	1	0	1.269432	-0.095637	-1.464032
3	1	0	0.674741	-1.260020	-0.270188
4	6	0	0.402121	0.803183	0.274246
5	1	0	0.354503	0.646173	1.358312
6	1	0	0.862225	1.771406	0.080693
7	7	0	-0.970214	0.894499	-0.279901
8	7	0	-1.714138	-0.055705	-0.013058
9	7	0	-2.516438	-0.867432	0.168081
10	7	0	2.559317	-0.316113	0.164606
11	1	0	2.537329	-0.691642	1.108403
12	1	0	3.145717	-0.943714	-0.376649

aga, E = -298.1522033 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.759115	0.475903	-0.154406
2	1	0	-1.854264	0.681022	-1.224773
3	1	0	-2.441901	1.149128	0.371755
4	6	0	-0.340884	0.810896	0.282051
5	1	0	-0.120627	1.869723	0.105596
6	1	0	-0.209247	0.587596	1.347040
7	7	0	0.583711	-0.027633	-0.524597
8	7	0	1.733443	-0.123520	-0.087131
9	7	0	2.835991	-0.285627	0.216742
10	7	0	-2.172667	-0.902872	0.093804
11	1	0	-1.508524	-1.532981	-0.347668
12	1	0	-2.128785	-1.097725	1.090448

agg, E = -298.15207 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.744107	0.490163	0.174751
2	1	0	1.827025	0.630687	1.261232
3	1	0	2.410355	1.210573	-0.307824
4	6	0	0.327360	0.812114	-0.248014
5	1	0	0.069166	1.841817	0.019984
6	1	0	0.218651	0.673692	-1.328934
7	7	0	-0.575527	-0.127096	0.469992
8	7	0	-1.745697	-0.140799	0.078781
9	7	0	-2.863100	-0.244603	-0.195061
10	7	0	2.106533	-0.856195	-0.271166
11	1	0	3.064685	-1.057746	-0.000617
12	1	0	1.525852	-1.531827	0.217918

***agg*⁻**, E = -298.1502115 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.728030	0.497168	-0.164737
2	1	0	-1.770153	0.683120	-1.241318
3	1	0	-2.369387	1.241425	0.327148
4	6	0	-0.312267	0.738970	0.317757
5	1	0	-0.067609	1.803822	0.242546
6	1	0	-0.211499	0.427806	1.364389
7	7	0	0.624283	-0.039208	-0.531495
8	7	0	1.774400	-0.135602	-0.096372
9	7	0	2.879121	-0.297743	0.201378
10	7	0	-2.139516	-0.884690	0.087611
11	1	0	-2.255331	-1.024225	1.087779
12	1	0	-3.052261	-1.048079	-0.326520

gga, E = -298.1522917 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.318232	-0.042718	0.679188
2	1	0	0.708133	-0.686033	1.322261
3	1	0	2.080690	0.416410	1.316040
4	6	0	0.445871	1.073974	0.112677
5	1	0	0.027837	1.686994	0.919718
6	1	0	1.026530	1.713538	-0.553328
7	7	0	-0.653415	0.537253	-0.732457
8	7	0	-1.528667	-0.085030	-0.121218
9	7	0	-2.414144	-0.678031	0.326286
10	7	0	1.981243	-0.879891	-0.317571
11	1	0	1.287352	-1.273494	-0.947023
12	1	0	2.589722	-0.305060	-0.894135

ggg, E = -298.1521449 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.324666	-0.005728	0.660475
2	1	0	0.725735	-0.646394	1.324663
3	1	0	2.097399	0.468217	1.272910
4	6	0	0.436670	1.090258	0.099037
5	1	0	0.014766	1.698379	0.906124
6	1	0	1.005077	1.729829	-0.575781
7	7	0	-0.662220	0.530617	-0.734307
8	7	0	-1.522238	-0.100269	-0.109973
9	7	0	-2.393797	-0.703584	0.350552
10	7	0	1.972747	-0.737902	-0.428722
11	1	0	2.562352	-1.469636	-0.042932
12	1	0	1.265215	-1.209603	-0.984907

ggg^{-}, E = -298.1510493 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.279349	-0.061932	0.638882
2	1	0	0.664587	-0.662200	1.317379
3	1	0	2.119626	0.332686	1.227410
4	6	0	0.479182	1.136904	0.155359
5	1	0	0.180076	1.751091	1.011659
6	1	0	1.073538	1.752917	-0.520961
7	7	0	-0.725777	0.764697	-0.628776
8	7	0	-1.461931	-0.073994	-0.103797
9	7	0	-2.229044	-0.853325	0.271618
10	7	0	1.685203	-0.910903	-0.481105
11	1	0	2.329353	-0.398767	-1.077717
12	1	0	2.202480	-1.710885	-0.128803

g^{-}***ga***, E = -298.1516445 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.686522	-0.129976	-0.120177
2	1	0	1.914255	-0.376784	-1.160704
3	1	0	2.577464	-0.355450	0.475314
4	6	0	0.568179	-1.047326	0.370011
5	1	0	0.868780	-2.091613	0.267360
6	1	0	0.338718	-0.848476	1.423197
7	7	0	-0.661697	-0.900749	-0.448646
8	7	0	-1.457251	-0.031509	-0.078151
9	7	0	-2.299544	0.718296	0.175197
10	7	0	1.415746	1.301562	-0.038950
11	1	0	0.665144	1.562062	-0.670004
12	1	0	1.126656	1.560864	0.899685

g^{-}***gg***, E = -298.151703 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.671630	-0.124268	-0.098625

2	1	0	1.957446	-0.364588	-1.130639
3	1	0	2.541713	-0.301598	0.540500
4	6	0	0.575054	-1.077921	0.345730
5	1	0	0.881377	-2.112555	0.185875
6	1	0	0.346670	-0.928915	1.406119
7	7	0	-0.657015	-0.897153	-0.464229
8	7	0	-1.439798	-0.026601	-0.070192
9	7	0	-2.271643	0.729167	0.198761
10	7	0	1.235288	1.264503	0.073071
11	1	0	2.043904	1.878013	0.081302
12	1	0	0.680959	1.553364	-0.727665

g⁻gg⁻, E = -298.1524594 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.620390	-0.116887	-0.209676
2	1	0	1.690604	-0.281616	-1.287959
3	1	0	2.594130	-0.367819	0.234926
4	6	0	0.590140	-1.076638	0.362854
5	1	0	0.921929	-2.106812	0.230541
6	1	0	0.445899	-0.893543	1.434571
7	7	0	-0.709230	-0.989886	-0.341099
8	7	0	-1.423882	-0.019751	-0.071289
9	7	0	-2.217872	0.802352	0.099438
10	7	0	1.202399	1.266382	0.020927
11	1	0	1.315955	1.497601	1.004249
12	1	0	1.808402	1.899658	-0.491237

2-Azidoethylammonium ion

aa, E = -298.5986324 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.480112	0.533831	-0.049335
2	1	0	1.545212	1.232773	0.783113
3	1	0	1.483256	1.079035	-0.991606
4	6	0	0.248090	-0.345068	0.069320
5	1	0	0.184218	-1.032172	-0.781300
6	1	0	0.271333	-0.922668	0.999861
7	7	0	-0.893379	0.588627	0.072938
8	7	0	-2.004668	0.048493	-0.001470
9	7	0	-3.094188	-0.321729	-0.065098
10	7	0	2.715112	-0.307281	-0.019333
11	1	0	2.808355	-0.817130	0.862303
12	1	0	2.723545	-0.996289	-0.775221
13	1	0	3.554732	0.267100	-0.126316

ag, E = -298.5985211 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.149971	-0.312178	-0.403880
2	1	0	1.232269	-0.095149	-1.467777
3	1	0	0.728377	-1.307105	-0.263863
4	6	0	0.321094	0.753784	0.303673
5	1	0	0.229804	0.535649	1.372916
6	1	0	0.776038	1.736864	0.181198
7	7	0	-1.005590	0.847408	-0.330038
8	7	0	-1.804543	-0.048801	-0.018157
9	7	0	-2.653373	-0.801215	0.187496
10	7	0	2.539865	-0.346555	0.149893
11	1	0	3.026289	0.542473	0.007904
12	1	0	2.547557	-0.546917	1.153195
13	1	0	3.098760	-1.071308	-0.306682

ga, E = -298.6032676 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.684750	0.580787	-0.190551
2	1	0	-1.788964	0.689460	-1.269086
3	1	0	-2.391584	1.234143	0.318265
4	6	0	-0.266337	0.859414	0.253963
5	1	0	0.004961	1.874372	-0.050335
6	1	0	-0.173169	0.773735	1.341982
7	7	0	0.582168	-0.145018	-0.422967
8	7	0	1.770120	-0.150686	-0.075308
9	7	0	2.893224	-0.252963	0.159268
10	7	0	-2.042031	-0.831847	0.141084
11	1	0	-1.342930	-1.469659	-0.252273
12	1	0	-2.069085	-0.989606	1.151117
13	1	0	-2.957073	-1.090045	-0.234679

gg, E = -298.6023669 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.301280	0.153715	0.718438
2	1	0	0.778428	-0.474627	1.439174
3	1	0	2.089363	0.710159	1.224841
4	6	0	0.347541	1.088340	-0.005588
5	1	0	-0.126202	1.749500	0.725210
6	1	0	0.879199	1.699587	-0.735529
7	7	0	-0.654728	0.320830	-0.777035
8	7	0	-1.597969	-0.130456	-0.108273
9	7	0	-2.532568	-0.592562	0.383043
10	7	0	1.951318	-0.763585	-0.267264
11	1	0	1.242453	-1.240281	-0.832857
12	1	0	2.566221	-0.257515	-0.908733
13	1	0	2.515237	-1.478745	0.197491

2-Azidoethanol

aaa, E = -318.0016906 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.583430	0.475376	-0.082047
2	1	0	-1.556153	0.976955	-1.054604
3	1	0	-1.629156	1.233516	0.707305
4	6	0	-0.332892	-0.360823	0.095884
5	1	0	-0.389809	-0.922769	1.033699
6	1	0	-0.223634	-1.060332	-0.738687
7	7	0	0.811207	0.578650	0.139013
8	7	0	1.923576	0.061722	-0.000138
9	7	0	3.015288	-0.296378	-0.112976
10	1	0	-3.475475	0.067230	-0.238726
11	8	0	-2.684792	-0.423734	0.003337

aag, E = -318.0020193 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.592951	0.492112	-0.050541
2	1	0	-1.568082	1.074614	-0.972424
3	1	0	-1.644519	1.181569	0.798841
4	6	0	-0.335567	-0.355029	0.055191
5	1	0	-0.365702	-0.973226	0.959467
6	1	0	-0.249056	-1.005188	-0.821140
7	7	0	0.812207	0.579508	0.126349
8	7	0	1.924116	0.056750	0.005472
9	7	0	3.015497	-0.307298	-0.091209
10	1	0	-2.843783	-0.779775	0.720216
11	8	0	-2.752562	-0.327902	-0.124642

gaa, E = -318.0020257 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.222013	-0.345788	0.360054
2	1	0	-1.289741	-0.176626	1.439676
3	1	0	-0.722865	-1.306168	0.183714
4	6	0	-0.420637	0.778988	-0.273730
5	1	0	-0.348889	0.634037	-1.356619
6	1	0	-0.896233	1.738478	-0.073984
7	7	0	0.929442	0.868059	0.326201
8	7	0	1.707532	-0.043278	0.019786
9	7	0	2.539286	-0.816638	-0.189755
10	1	0	-3.055102	-0.968418	0.205471
11	8	0	-2.508137	-0.322188	-0.251228

gag, E = -318.0023316 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.224686	-0.336646	-0.390570
2	1	0	1.287083	-0.130013	-1.459931
3	1	0	0.724834	-1.302460	-0.251344
4	6	0	0.427473	0.768914	0.293202
5	1	0	0.362423	0.589175	1.372473
6	1	0	0.906293	1.732928	0.125082
7	7	0	-0.928982	0.884649	-0.288625
8	7	0	-1.706151	-0.038201	-0.015976
9	7	0	-2.538312	-0.818048	0.167246
10	1	0	2.527560	-0.651505	1.015428
11	8	0	2.561621	-0.378817	0.092998

***gag*⁻**, E = -318.0023218 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.214669	-0.369888	0.357948
2	1	0	-1.260022	-0.211940	1.440610
3	1	0	-0.718816	-1.324316	0.167534
4	6	0	-0.428278	0.764906	-0.289809
5	1	0	-0.360083	0.609594	-1.371413
6	1	0	-0.913142	1.723411	-0.101404
7	7	0	0.922580	0.882884	0.305523
8	7	0	1.708181	-0.028921	0.020569
9	7	0	2.545907	-0.800511	-0.172014
10	1	0	-3.007495	0.306767	0.043201
11	8	0	-2.514930	-0.480974	-0.208238

aga, E = -318.0033601 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.736587	0.465346	0.194600
2	1	0	1.777256	0.544331	1.286145
3	1	0	2.395765	1.225115	-0.240195
4	6	0	0.329865	0.736264	-0.276307
5	1	0	0.075864	1.784482	-0.086117
6	1	0	0.253232	0.535130	-1.350245
7	7	0	-0.595033	-0.146660	0.475308
8	7	0	-1.765387	-0.138465	0.084014
9	7	0	-2.885923	-0.220205	-0.184092
10	1	0	2.959188	-1.043640	0.160899
11	8	0	2.108049	-0.839721	-0.238357

agg, E = -318.0032141 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.751429	0.457467	-0.167869
2	1	0	-1.820435	0.622614	-1.244426
3	1	0	-2.427059	1.157773	0.336257

4	6	0	-0.339636	0.742684	0.299640
5	1	0	-0.120901	1.808643	0.169326
6	1	0	-0.230523	0.487396	1.360158
7	7	0	0.596914	-0.065404	-0.516077
8	7	0	1.753502	-0.124457	-0.089666
9	7	0	2.863352	-0.256269	0.201384
10	1	0	-2.148091	-1.038534	1.002976
11	8	0	-2.150371	-0.889486	0.051949

***agg*⁻**, E = -318.0051665 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.773161	0.425975	0.145928
2	1	0	1.898783	0.574648	1.224434
3	1	0	2.490138	1.056925	-0.381834
4	6	0	0.369737	0.823479	-0.257449
5	1	0	0.187091	1.877414	-0.023313
6	1	0	0.225918	0.651790	-1.328928
7	7	0	-0.556916	-0.035754	0.523301
8	7	0	-1.708864	-0.112355	0.085198
9	7	0	-2.812301	-0.259448	-0.219732
10	1	0	1.384068	-1.461051	0.199127
11	8	0	2.062897	-0.917943	-0.217716

gga, E = -318.0033804 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.309960	-0.112218	0.630325
2	1	0	0.695330	-0.838340	1.175987
3	1	0	2.081304	0.266236	1.311510
4	6	0	0.458832	1.057897	0.185896
5	1	0	0.092168	1.599698	1.064488
6	1	0	1.047519	1.738567	-0.428661
7	7	0	-0.682441	0.647609	-0.668146
8	7	0	-1.516983	-0.076742	-0.116422
9	7	0	-2.367522	-0.753782	0.275297
10	1	0	2.317651	-1.520406	-0.247102
11	8	0	1.890238	-0.704927	-0.526082

ggg, E = -318.0035865 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.303872	-0.126116	0.636230
2	1	0	0.687364	-0.788732	1.248438
3	1	0	2.132042	0.236292	1.256686
4	6	0	0.493345	1.075901	0.180465
5	1	0	0.163598	1.646040	1.056768
6	1	0	1.094407	1.729026	-0.453212
7	7	0	-0.675017	0.702046	-0.651513

8	7	0	-1.487479	-0.056430	-0.113214
9	7	0	-2.322115	-0.758406	0.268968
10	1	0	2.346421	-0.365932	-0.983281
11	8	0	1.773142	-0.920734	-0.444407

***ggg*⁻**, E = -318.0047786 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.348709	-0.054034	0.658528
2	1	0	0.756472	-0.716523	1.302351
3	1	0	2.141807	0.392360	1.261787
4	6	0	0.467440	1.048742	0.100721
5	1	0	0.050208	1.655445	0.911805
6	1	0	1.043013	1.686309	-0.569686
7	7	0	-0.622910	0.486281	-0.738492
8	7	0	-1.525646	-0.081891	-0.111357
9	7	0	-2.435565	-0.623883	0.349305
10	1	0	1.292331	-1.117676	-0.956138
11	8	0	1.988515	-0.791464	-0.375226

g*⁻*ga, E = -318.0052708 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.609351	-0.020478	-0.200778
2	1	0	1.700485	-0.141963	-1.285151
3	1	0	2.591882	-0.169590	0.262151
4	6	0	0.652651	-1.056842	0.345530
5	1	0	1.048188	-2.056454	0.166071
6	1	0	0.517768	-0.916234	1.423569
7	7	0	-0.657356	-1.017470	-0.341277
8	7	0	-1.388615	-0.059639	-0.066450
9	7	0	-2.189599	0.754772	0.104724
10	1	0	1.624435	1.922920	-0.304556
11	8	0	1.074277	1.260200	0.123803

g*⁻*gg, E = -318.0051014 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.602424	-0.009868	-0.231407
2	1	0	1.665420	-0.149533	-1.311713
3	1	0	2.600214	-0.142727	0.202386
4	6	0	0.662888	-1.045986	0.360058
5	1	0	1.064893	-2.047301	0.200742
6	1	0	0.539693	-0.884776	1.437514
7	7	0	-0.656804	-1.034922	-0.306745
8	7	0	-1.386554	-0.067899	-0.061680
9	7	0	-2.188931	0.749678	0.088792
10	1	0	1.205643	1.514195	0.906694
11	8	0	1.119787	1.314659	-0.031262

Protonated 2-azidoethanol

aaa, E = -318.3950331 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.460695	0.534068	0.103773
2	1	0	-1.573957	1.288510	-0.669790
3	1	0	-1.471382	0.983010	1.092884
4	6	0	-0.262542	-0.364435	-0.128796
5	1	0	-0.165313	-1.097588	0.677169
6	1	0	-0.345926	-0.880476	-1.090201
7	7	0	0.873837	0.573861	-0.141429
8	7	0	1.984741	0.045574	0.000766
9	7	0	3.072790	-0.312437	0.119796
10	1	0	-2.902899	-0.669372	-0.814391
11	1	0	-2.842641	-0.894599	0.755014
12	8	0	-2.734754	-0.237034	0.043190

aag, E = -318.3953944 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.457020	0.530934	0.080711
2	1	0	-1.575770	1.247412	-0.728444
3	1	0	-1.466699	1.014663	1.052913
4	6	0	-0.259749	-0.376045	-0.100886
5	1	0	-0.155997	-1.038478	0.762461
6	1	0	-0.356613	-0.971918	-1.013865
7	7	0	0.875324	0.556699	-0.212657
8	7	0	1.985759	0.049733	-0.005222
9	7	0	3.073383	-0.290498	0.160708
10	1	0	-3.447455	0.083195	0.485586
11	1	0	-2.912888	-0.686278	-0.787503
12	8	0	-2.665653	-0.348684	0.093763

gaa, E = -318.3952158 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.169850	-0.266679	-0.453387
2	1	0	1.332420	0.072804	-1.472441
3	1	0	0.784194	-1.283267	-0.438031
4	6	0	0.331890	0.706427	0.360262
5	1	0	0.219305	0.367174	1.393973
6	1	0	0.774668	1.701779	0.352531
7	7	0	-0.971356	0.832002	-0.314980
8	7	0	-1.804302	-0.041352	-0.021109
9	7	0	-2.681604	-0.763410	0.167589
10	1	0	3.085450	0.402295	0.078357
11	1	0	2.585447	-0.785149	1.003338

12	8	0	2.551114	-0.413101	0.102566

gag, E = -318.3954753 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.154490	-0.275619	0.431747
2	1	0	-1.320747	-0.004673	1.471507
3	1	0	-0.755413	-1.282514	0.338522
4	6	0	-0.329669	0.748015	-0.326836
5	1	0	-0.238327	0.466932	-1.379181
6	1	0	-0.771675	1.741045	-0.251797
7	7	0	0.984047	0.837641	0.334274
8	7	0	1.793280	-0.050570	0.019222
9	7	0	2.650229	-0.792236	-0.187309
10	1	0	-2.969880	-1.188959	-0.026393
11	1	0	-3.083799	0.385400	-0.037406
12	8	0	-2.493512	-0.364432	-0.238503

***gag*$^-$**, E = -318.3956429 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.174159	-0.267475	-0.440487
2	1	0	1.341257	0.073389	-1.458499
3	1	0	0.805476	-1.290882	-0.416129
4	6	0	0.325050	0.710787	0.350438
5	1	0	0.210003	0.391405	1.390204
6	1	0	0.776146	1.701452	0.322932
7	7	0	-0.976884	0.821573	-0.328792
8	7	0	-1.808486	-0.049275	-0.025021
9	7	0	-2.684670	-0.771009	0.170366
10	1	0	2.599357	-0.793272	0.999113
11	1	0	3.233907	-0.585767	-0.432287
12	8	0	2.541111	-0.270652	0.177385

aga, E = -318.4016294 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.734825	0.532579	-0.147776
2	1	0	-1.925248	0.650867	-1.210690
3	1	0	-2.503776	1.009871	0.452477
4	6	0	-0.326588	0.917319	0.239067
5	1	0	-0.124515	1.929067	-0.123108
6	1	0	-0.187499	0.876729	1.322994
7	7	0	0.519055	-0.088893	-0.440469
8	7	0	1.703922	-0.122077	-0.073402
9	7	0	2.820659	-0.237193	0.173555
10	1	0	-1.008318	-1.346872	-0.145208
11	1	0	-2.123178	-1.178576	0.983391
12	8	0	-1.883055	-0.937917	0.069326

agg, E = -318.402537 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.727943	0.541171	-0.160187
2	1	0	-1.904902	0.596801	-1.232036
3	1	0	-2.483157	1.068788	0.414403
4	6	0	-0.318455	0.914313	0.221552
5	1	0	-0.101767	1.915824	-0.159274
6	1	0	-0.194195	0.892358	1.307715
7	7	0	0.521735	-0.116237	-0.428170
8	7	0	1.711024	-0.130551	-0.075036
9	7	0	2.830984	-0.234750	0.162606
10	1	0	-2.639086	-1.336999	-0.129292
11	1	0	-1.033978	-1.353025	-0.072720
12	8	0	-1.851341	-0.893235	0.235901

agg^{-}, E = -318.3989511 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.659204	0.583900	-0.195853
2	1	0	-1.733749	0.648305	-1.277966
3	1	0	-2.364824	1.244313	0.302797
4	6	0	-0.255508	0.772164	0.300431
5	1	0	-0.005554	1.825969	0.131957
6	1	0	-0.189160	0.571462	1.375418
7	7	0	0.625052	-0.118338	-0.472726
8	7	0	1.801039	-0.146119	-0.085919
9	7	0	2.917907	-0.266982	0.169185
10	1	0	-2.101468	-1.029241	1.053466
11	1	0	-2.941329	-1.056384	-0.282598
12	8	0	-2.072954	-0.827592	0.099460

gga, E = -318.4004896 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.431130	0.395495	0.623288
2	1	0	1.034545	0.087784	1.587472
3	1	0	2.335732	0.987596	0.734940
4	6	0	0.384988	1.017022	-0.281619
5	1	0	-0.120903	1.828269	0.246956
6	1	0	0.836913	1.405113	-1.194116
7	7	0	-0.538150	-0.065430	-0.698305
8	7	0	-1.601989	-0.142333	-0.057817
9	7	0	-2.627297	-0.304751	0.435670
10	1	0	1.044433	-1.261558	-0.450900
11	1	0	2.552462	-0.790440	-0.674882
12	8	0	1.849020	-0.893033	-0.007040

ggg, E = -318.4013404 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.433391	0.386638	0.619621
2	1	0	1.043967	0.017288	1.566697
3	1	0	2.318894	1.002631	0.749664
4	6	0	0.374588	1.024769	-0.254212
5	1	0	-0.129056	1.816318	0.304875
6	1	0	0.822946	1.442982	-1.155002
7	7	0	-0.548970	-0.045191	-0.700053
8	7	0	-1.605641	-0.147651	-0.052219
9	7	0	-2.625747	-0.331561	0.444976
10	1	0	2.420551	-1.432788	0.343032
11	1	0	1.072521	-1.246971	-0.511470
12	8	0	1.883102	-0.799635	-0.167397

***ggg*⁻**, E = -318.3982644 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.263306	0.024150	0.727397
2	1	0	0.733260	-0.756506	1.268190
3	1	0	2.046516	0.470203	1.337375
4	6	0	0.349857	1.059673	0.119082
5	1	0	-0.077699	1.633279	0.949013
6	1	0	0.909818	1.749587	-0.512474
7	7	0	-0.692421	0.471119	-0.736140
8	7	0	-1.603407	-0.111286	-0.128290
9	7	0	-2.514111	-0.673754	0.299127
10	1	0	2.541845	-0.162987	-0.912582
11	1	0	2.413265	-1.508092	-0.095073
12	8	0	1.927948	-0.716372	-0.394525

***g*⁻*gg*⁻**, E = -318.3986268 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.621842	-0.230298	-0.180272
2	1	0	1.717019	-0.328260	-1.258012
3	1	0	2.573183	-0.370793	0.329326
4	6	0	0.519153	-1.093430	0.378559
5	1	0	0.849400	-2.128220	0.274299
6	1	0	0.357851	-0.893927	1.442745
7	7	0	-0.725579	-0.965755	-0.394758
8	7	0	-1.460621	-0.019724	-0.073127
9	7	0	-2.248323	0.797901	0.125284
10	1	0	1.339632	1.527316	0.923388
11	1	0	1.664630	1.818220	-0.595524
12	8	0	1.211747	1.203884	0.011533

N-(2-Azidoathyl)ethanamide

aag, E = -450.5143881 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.124481	0.908233	-0.577796
2	1	0	-0.165560	1.954897	-0.684342
3	1	0	0.199320	0.459378	-1.570743
4	6	0	-0.915027	0.156529	0.242079
5	1	0	-0.601263	-0.882644	0.379225
6	1	0	-1.039690	0.632586	1.220350
7	7	0	-2.186392	0.204952	-0.519799
8	7	0	-3.182190	-0.186741	0.096675
9	7	0	-4.183545	-0.525551	0.561266
10	7	0	1.424211	0.854132	0.059699
11	1	0	1.709895	1.615645	0.656849
12	6	0	2.230351	-0.232458	-0.052752
13	6	0	3.539498	-0.164173	0.696859
14	1	0	3.686890	0.785434	1.212992
15	1	0	3.565169	-0.977285	1.425566
16	1	0	4.354647	-0.320116	-0.012551
17	8	0	1.913773	-1.213029	-0.732821

gag, E = -450.5150715 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.102552	-0.747450	-0.685175
2	1	0	0.361430	-1.573423	-1.349917
3	1	0	0.352604	0.193728	-1.182320
4	6	0	0.879845	-0.866223	0.625850
5	1	0	0.577163	-0.072812	1.316259
6	1	0	0.694974	-1.834574	1.090247
7	7	0	2.340749	-0.809856	0.386682
8	7	0	2.769817	0.296523	0.037085
9	7	0	3.303368	1.270037	-0.282413
10	7	0	-1.326019	-0.772137	-0.446635
11	1	0	-1.820890	-1.649042	-0.514871
12	6	0	-1.992640	0.333760	-0.026189
13	6	0	-3.470078	0.159027	0.230636
14	1	0	-3.820403	-0.855199	0.034845
15	1	0	-3.674290	0.415821	1.272240
16	1	0	-4.017976	0.858874	-0.403684
17	8	0	-1.423262	1.418747	0.125428

gag^{-}, E = -450.5147341 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.160779	-0.350143	-0.513802
2	1	0	-0.079878	0.333635	-1.361464
3	1	0	-0.731853	-1.227904	-0.825409

4	6	0	-0.860046	0.360518	0.644904
5	1	0	-0.964904	-0.314802	1.500851
6	1	0	-0.283159	1.233580	0.946343
7	7	0	-2.184654	0.879635	0.233711
8	7	0	-3.047470	0.018620	0.023753
9	7	0	-3.947036	-0.672848	-0.193576
10	7	0	1.167009	-0.785554	-0.131961
11	1	0	1.294817	-1.724429	0.215189
12	6	0	2.218362	0.073802	-0.108588
13	6	0	3.533904	-0.504469	0.355350
14	1	0	3.466326	-1.560229	0.621284
15	1	0	4.268317	-0.380460	-0.443241
16	1	0	3.877383	0.064366	1.221900
17	8	0	2.106170	1.252378	-0.458265

agg, E = -450.5162202 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.228328	-1.447832	-0.446824
2	1	0	-0.084613	-1.927831	-1.376116
3	1	0	0.773084	-2.176545	0.157194
4	6	0	-0.987026	-0.978976	0.334233
5	1	0	-1.636022	-1.830556	0.565849
6	1	0	-0.671510	-0.496984	1.264800
7	7	0	-1.709766	-0.005110	-0.520166
8	7	0	-2.698135	0.520014	0.001167
9	7	0	-3.637210	1.079672	0.373817
10	7	0	1.121683	-0.355612	-0.776498
11	1	0	0.965891	0.149619	-1.636048
12	6	0	1.962162	0.179347	0.145567
13	6	0	2.727497	1.404985	-0.293483
14	1	0	2.606108	1.624423	-1.355211
15	1	0	2.376266	2.259296	0.290478
16	1	0	3.785706	1.255771	-0.071778
17	8	0	2.095415	-0.309386	1.271956

***agg*$^{-}$**, E = -450.515454 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.223329	1.558799	0.177825
2	1	0	0.353996	1.435911	1.253421
3	1	0	0.397720	2.607579	-0.078947
4	6	0	-1.195176	1.190714	-0.219778
5	1	0	-1.903546	1.842478	0.303457
6	1	0	-1.333581	1.306414	-1.300701
7	7	0	-1.420276	-0.223932	0.161372
8	7	0	-2.573462	-0.631530	-0.005494
9	7	0	-3.609325	-1.129776	-0.119860
10	7	0	1.205695	0.724572	-0.481454
11	1	0	1.329992	0.826929	-1.478499
12	6	0	1.898196	-0.256767	0.152993

13	6	0	2.811998	-1.076625	-0.728544
14	1	0	2.884116	-0.691685	-1.746735
15	1	0	3.805802	-1.099065	-0.277705
16	1	0	2.431768	-2.100551	-0.759969
17	8	0	1.798152	-0.475009	1.363594

ggg, E = -450.5161536 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.145934	0.728827	0.923931
2	1	0	-0.834053	0.374250	1.695427
3	1	0	0.384520	1.601211	1.314724
4	6	0	-0.912262	1.150120	-0.325394
5	1	0	-1.593929	1.974087	-0.086864
6	1	0	-0.219539	1.472753	-1.100675
7	7	0	-1.666292	0.019410	-0.918882
8	7	0	-2.607586	-0.404018	-0.238893
9	7	0	-3.513071	-0.890386	0.289366
10	7	0	0.812073	-0.325300	0.657582
11	1	0	0.544948	-1.284005	0.823161
12	6	0	1.987030	-0.073626	0.027436
13	6	0	2.848909	-1.277392	-0.270122
14	1	0	2.449820	-2.201251	0.150737
15	1	0	2.932190	-1.384352	-1.354243
16	1	0	3.848760	-1.098731	0.129869
17	8	0	2.330620	1.072566	-0.278933

***ggg*$^-$**, E = -450.5173091 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.138400	1.371474	-0.773791
2	1	0	0.382335	0.637296	-1.544549
3	1	0	0.016708	2.346333	-1.254043
4	6	0	1.269266	1.464734	0.246085
5	1	0	2.191395	1.788306	-0.250164
6	1	0	1.019148	2.181706	1.028272
7	7	0	1.488805	0.181509	0.952259
8	7	0	1.938220	-0.733166	0.253365
9	7	0	2.362470	-1.666560	-0.278282
10	7	0	-1.116330	0.976913	-0.169343
11	1	0	-1.646741	1.670175	0.338050
12	6	0	-1.545327	-0.311680	-0.146609
13	6	0	-2.828476	-0.558252	0.611793
14	1	0	-3.325467	0.362046	0.921949
15	1	0	-3.501970	-1.140612	-0.019406
16	1	0	-2.595830	-1.153637	1.498168
17	8	0	-0.931863	-1.225019	-0.706143

g*$^-$*gg, E = -450.5178264 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.296952	-1.564350	0.589073
2	1	0	0.752330	-1.832506	1.543695
3	1	0	-0.251881	-2.429095	0.204017
4	6	0	1.384635	-1.189404	-0.412793
5	1	0	2.085477	-2.017019	-0.525279
6	1	0	0.945084	-0.956837	-1.386729
7	7	0	2.188900	-0.041784	0.068626
8	7	0	1.672529	1.071898	-0.079481
9	7	0	1.331629	2.171574	-0.184473
10	7	0	-0.623750	-0.469666	0.829227
11	1	0	-0.571241	0.033592	1.702375
12	6	0	-1.559789	-0.103424	-0.083954
13	6	0	-2.393353	1.101388	0.279983
14	1	0	-2.366107	1.327017	1.347112
15	1	0	-2.008757	1.964266	-0.271320
16	1	0	-3.423642	0.927636	-0.032615
17	8	0	-1.689636	-0.700809	-1.156550

***g*⁻*gg*⁻**, E = -450.5178436 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.639804	-1.629832	-0.049988
2	1	0	0.483335	-1.763112	1.021153
3	1	0	0.734476	-2.613370	-0.519632
4	6	0	1.922960	-0.841355	-0.288564
5	1	0	2.776963	-1.402212	0.092359
6	1	0	2.070164	-0.656216	-1.358530
7	7	0	1.930576	0.440016	0.450597
8	7	0	1.177282	1.324151	0.027723
9	7	0	0.558279	2.257731	-0.260607
10	7	0	-0.522713	-0.948770	-0.583130
11	1	0	-0.678387	-0.973275	-1.580909
12	6	0	-1.425647	-0.289200	0.192073
13	6	0	-2.531438	0.408221	-0.562724
14	1	0	-2.649427	0.037870	-1.582310
15	1	0	-3.467028	0.285307	-0.015886
16	1	0	-2.293496	1.475235	-0.601008
17	8	0	-1.326830	-0.223641	1.419737