Non-planarity at Tri-coordinated Aluminum and Gallium:

Cyclic Structures for $X_3H_n^m$ (X=B, Al, Ga)

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Supplementary material

Tables of Total Energies and Cartesian coordinates of the structures in Figures 1-4.

Table 1.

Total energy (in au) and Zero point energy (ZPE, in kcal/mol) of the calculated $X_3H_3^{2-}$ isomers at B3LYP and HF levels using 6-311G(d) basis.

X	Structure	Total Energy B3LYP	ZPE	Total Energy HF	ZPE
B	1a	-76.13605(0)	19.56	-75.49506(0)	20.43
	1b	--	--	--	--
	1c	-76.04298(0)	19.27	-75.39855(0)	20.54
	1d	-75.98810(3)	14.92	-75.31609(3)	16.36
	1e	-75.98920(2)	15.59	-75.33537(0)	19.18
	1f	-76.07366(1)	18.26	-75.42791(0)	19.85
	1g	Collapsed to 1a		--	--
	1h	-76.01688(3)	18.51	-75.36445(3)	19.50
	1i	--	--	--	--
	1j	-75.98452(2)	16.05	-75.34209(2)	17.04
	1k	-76.04195(1)	18.17	-75.39221(1)	19.38
Al	1a	-729.05334(0)	11.05	-727.33170(0)	12.17
	1b	--	--	--	--
	1c	-729.05814(0)	12.29	-727.33364(0)	13.01
	1d	-729.03639(1)	11.60	-727.30656(1)	12.43
	1e	-729.04584(0)	12.50	-727.32263(0)	13.40
	1f	-729.05615(0)	11.66	-727.33140(0)	12.58
	1g	-729.05151(0)	11.74	-727.32938(0)	12.63
	1h	-729.03369(2)	12.00	-727.30792(2)	12.74
	1i	-729.04896(0)	12.08	-727.32481(0)	12.93
	1j	-729.02153(1)	10.91	-727.30195(0)	12.16
	1k	-729.05104(0)	11.66	-727.32215(0)	12.45
Ga	1a	-5776.32355(1)	9.30	-5771.20605(0)	11.02
	1b	-5776.32355(0)	9.48	Collapsed to 1a	
	1c	-5776.33704(0)	10.98	-5771.21505(0)	11.71
	1d	-5776.31874(1)	10.52	-5771.18718(1)	10.78
	1e	-5776.32482(0)	10.32	-5771.19921(0)	10.99
	1f	-5776.32939(0)	10.28	-5771.20745(0)	10.97
	1g	-5776.32891(0)	10.55	Collapsed to open chain	
	1h	-5776.30626(1)	17.99	-5771.19418(1)	9.59
	1i	-5776.32797(0)	10.55	-5771.20433(0)	11.15
	1j	-5776.30054(1)	9.40	-5771.18112(0)	10.02
	1k	-5776.32268(0)	9.13	-5771.19436(1)	9.69

Table 2.

Total energy (in au) and Zero point energy (ZPE, in kcal/mol) of the calculated $X_3H_4^-$ isomers at B3LYP and HF levels using 6-311G(d) basis.

X	Structure	Total Energy B3LYP	ZPE	Total Energy HF	ZPE
B	2a	-76.94825(0)	27.39	-76.30896(0)	28.65
	2b	--		--	
	2c	Collapsed to 2a		--	
	2d	Collapsed to 2a		--	
	2e	-76.94432(0)	26.56	-76.30513(0)	28.03
	2f	-76.86692(2)	23.56	-76.23969(2)	24.82
	2g	--		--	
	2h	-76.87374(1)	25.42	-76.23057(1)	26.88
	2i	--		--	
	2j	-76.81261(2)	23.57	-76.17911(1)	25.46
	2k	--		--	
	2l	-76.90050(2)	23.46	-76.26657(0)	25.08
Al	2a	-729.77469(1)	16.94	-728.05603(1)	17.93
	2b	-729.77635(0)	16.96	-728.05649(0)	18.09
	2c	Collapsed to open chain		--	
	2d	-729.76814(0)	17.17	-728.04423(0)	18.10
	2e	-729.74222(2)	15.83	-728.02138(2)	16.77
	2f	-729.73719(2)	14.63	-727.98262(2)	16.34
	2g	-729.76166(0)	15.79	-728.03867(0)	16.62
	2h	-729.76241(2)	15.69	-728.03667(2)	16.44
	2i	-729.76495(0)	17.04	Collapsed	
	2j	-729.76100(1)	16.76	-727.92559(0)	18.08
	2k	-729.76169(0)	16.40	Collapsed to 2j	
	2l	-729.75594(0)	14.61	-728.03487(0)	15.59
Ga	2a	-5777.03364(1)	15.56	-5771.92189(1)	16.73
	2b	-5777.03703(0)	15.28	-5771.92209(0)	16.78
	2c	-5777.00133(1)	15.55	-5771.86933(1)	16.17
	2d	-5777.03947(0)	15.17	-5771.91661(1)	15.44
	2e	-5777.01165(2)	15.91	-5771.89775(2)	14.41
	2f	-5777.00188(3)	13.52	-5771.89639(2)	14.85
	2g	-5777.03459(0)	15.18	-5771.91562(0)	15.89
	2h	-5777.03620(2)	15.37	-5771.91727(2)	16.01
	2i	-5777.03455(0)	15.60	Collapsed	
	2j	-5777.02480(1)	14.86	-5771.90868(0)	15.99
	2k	-5777.02570(0)	14.46	Collapsed to 2j	
	2l^a	-5777.01450(0)	12.79	-5771.89682(1)	14.25

^aC₃ symmetry.

Table 3.

Total energy (in au) and Zero point energy (ZPE, in kcal/mol) of the calculated X_3H_5 isomers at B3LYP and HF levels using 6-311G(d) basis.

X	Structure	Total Energy B3LYP	ZPE	Total Energy HF	ZPE
B	3a	-77.51782(0)	34.21	-76.87666(0)	35.68
	3b	--		--	
	3c	Collapsed to 3j		--	
	3d	--		--	
	3e	--		--	
	3f	Collapsed to 3i		--	
	3g	Collapsed to 3i		--	
	3h	--		--	
	3i	--		--	
	3j	--		--	
	3k	-77.47429(0)	33.21	-76.84929(0)	35.08
	3l	-77.51758(0)	34.21	-76.87858(0)	36.03
	3m	-77.42558(2)	32.30	-76.79584(2)	34.22
	3n	--		--	
	3o	-77.42207(2)	30.39	-76.79243(2)	31.69
	3p	-77.39836(2)	30.97	-76.76280(2)	32.79
Al	3a	-730.29625(2)	22.55	-728.57656(2)	23.82
	3b	-730.32620(0)	22.70	-728.61132(0)	23.96
	3c	-730.31360(1)	21.20	-728.60292(1)	22.22
	3d	-730.32333(0)	22.40	-728.60756(0)	23.38
	3e	-730.32147(0)	22.29	-728.60756(0)	23.39
	3f	-730.25477(3)	21.71	-728.52154(3)	22.83
	3g	-730.31962(0)	22.31	-728.60183(0)	23.48
	3h	-730.31914(0)	22.04	Collapsed to open chain	
	3i	-730.32149(0)	22.87	Collapsed to open chain	
	3j	-730.31571(0)	21.92	-728.60272(0)	23.00
	3k	-730.32582(0)	22.62	-728.61752(0)	24.05
	3l	-730.27906(3)	21.04	-728.55857(3)	22.28
	3m	-730.30357(2)	20.12	-728.59810(0)	21.83
	3n	-730.30891(1)	21.23	-728.59811(0)	21.84
	3o	-730.28979(2)	19.46	-728.58763(1)	20.93
	3p	-730.27003(2)	19.66	-728.53484(2)	21.17

Continued.....

Table 3 (Continued)

X	Structure	Total Energy B3LYP	ZPE	Total Energy HF	ZPE
Ga	3a	-5777.53596(2)	21.58	-5772.42651(2)	22.72
	3b	-5777.57175(0)	21.04	-5772.46315(0)	21.94
	3c	-5777.58304(1)	19.89	-5772.47294(1)	20.58
	3d	-5777.58863(0)	20.73	-5772.47482(0)	21.14
	3e	Collapsed to 3d			
	3f	-5777.50939(3)	21.05	-5772.38410(3)	21.90
	3g	-5777.57670(0)	20.73	-5772.46532(0)	21.71
	3h	-5777.57988(0)	20.56	Collapsed to open chain	
	3i	-5777.57856(0)	21.28	Collapsed to open chain	
	3j	-5777.57664(0)	20.63	-5772.46821(1)	21.47
	3k	-5777.56954(0)	20.69	-5772.46645(0)	21.99
	3l	-5777.52681(2)	20.72	-5772.41419(2)	21.71
	3m	-5777.56377(1)	19.29	-5772.46323(1)	20.54
	3n	-5777.56445(0)	20.78	Collapsed	
	3o	-5777.55548(2)	19.12	-5772.46130(1)	20.34
	3p	-5777.50943(3)	17.73	-5772.37900(2)	19.57

Table 4.

Total energy (in au) and Zero point energy (ZPE, in kcal/mol) of the calculated $X_3H_6^+$ isomers at B3LYP and HF levels using 6-311G(d) basis.

X	Structure	Total Energy B3LYP	ZPE	Total Energy HF	ZPE
B	4a	-77.76101(1)	39.62	-77.10125(1)	42.17
	4b	-77.82878(0)	41.50	-77.20284(0)	43.60
	4c	--	--	--	--
	4d	--	--	--	--
	4e	-77.79360(2)	37.95	-77.17818(1)	40.39
	4f	--	--	--	--
	4g	-77.76097(2)	38.46	-77.14284(2)	40.33
	4h	-77.81388(0)	40.31	-77.19585(0)	42.48
	4i	-77.79924(1)	39.65	-77.18582(1)	41.74
	4j	-77.70196(3)	36.47	-77.10576(3)	38.46
	4k	-77.45232(4)	34.06	-76.76086(4)	36.00
Al	4a	-730.58422(3)	27.28	-728.85937(3)	28.89
	4b	-730.67944(0)	28.26	-728.97089(0)	29.89
	4c	-730.70348(0)	28.45	-729.00131(0)	29.63
	4d	-730.67887(1)	26.74	Collapsed	--
	4e	-730.67557(1)	27.06	-728.98151(1)	28.56
	4f	-730.69450(0)	28.51	-728.99437(0)	30.14
	4g	-730.65731(1)	26.19	-728.96047(1)	27.81
	4h	-730.65672(1)	26.94	-728.95226(1)	28.64
	4i	-730.65136(2)	26.89	-728.94775(2)	28.53
	4j	-730.60920(3)	24.36	-728.90687(3)	25.86
	4k	-730.50037(5)	23.28	-728.74077(5)	26.15
Ga	4a	-5777.80544(3)	26.18	-5772.69417(3)	28.03
	4b	-5777.90152(0)	26.00	-5772.80178(0)	27.52
	4c	-5777.94329(0)	26.91	-5772.84951(0)	27.83
	4d	Collapsed to open chain	--	--	--
	4e	-5777.91435(0)	25.96	-5772.82962(0)	27.18
	4f	-5777.92205(0)	26.78	-5772.83036(0)	27.91
	4g	-5777.90595(1)	25.66	-5772.81802(1)	27.03
	4h	-5777.88777(2)	25.42	-5772.79075(2)	26.67
	4i	-5777.88175(3)	25.24	-5772.78556(3)	26.45
	4j	-5777.86430(3)	24.28	-5772.77254(3)	25.52
	4k	-5777.82033(3)	23.84	-5772.66887(5)	26.23

Table 5.

Relative energies (in kcal/mol)^a of the calculated isomers for B, Al and Ga at B3LYP/6-311G(d) level. The values in parenthesis are number of imaginary frequencies.

	Structure	B	Al	Ga
$X_3H_3^{2-}$	1a	0.0(0)	0.0(0)	0.0(1)
	1b	--	--	0.18(0)
	1c	58.12(0)	-1.80(0)	-6.82(0)
	1d	88.29(3)	11.17(1)	4.21(1)
	1e	88.25(2)	6.13(0)	0.20(0)
	1f	37.87(1)	-1.16(0)	-2.70(0)
	1g	--	1.82(0)	-2.14(0)
	1h	73.75(3)	13.26(2)	19.37(1)
	1i	--	3.76(0)	-1.55(0)
	1j	91.64(2)	19.82(1)	14.54(1)
	1k	57.68(1)	2.04(0)	0.38(0)
$X_3H_4^-$	2a	0.0(0)	0.0(1)	0.0(1)
	2b	--	-1.02(0)	-2.40(0)
	2c	--	--	20.26(1)
	2d	--	4.34(0)	-4.04(0)
	2e	1.65(0)	19.29(2)	14.14(2)
	2f	47.29(2)	21.27(2)	17.93(3)
	2g	--	7.05(0)	-0.97(0)
	2h	44.82(1)	6.48(2)	-1.79(2)
	2i	--	6.21(0)	-0.53(0)
	2j	81.37(2)	8.41(1)	4.86(1)
	2k	--	7.63(0)	3.90(0)
	2l	26.11(2)	9.48(0)	8.79(0) ^b

Continued

Table 5. (Continued)

	Structure	B	Al	Ga
X_3H_5	3a	0.0(0)	0.0(2)	0.0(2)
	3b	--	-18.64(0)	-23.97(0)
	3c	--	-12.21(1)	-31.20(1)
	3d	--	-17.14(0)	-33.88(0)
	3e	--	-16.08(0)	--
	3f	--	25.20(3)	16.15(3)
	3g	--	-14.90(0)	-26.40(0)
	3h	--	-14.86(0)	-28.56(0)
	3i	--	-15.52(0)	-27.03(0)
	3j	--	-12.83(0)	-26.46(0)
	3k	26.33(0)	-18.49(0)	-21.94(0)
	3l	0.15(0)	9.31(3)	4.90(2)
	3m	56.00(2)	-6.98(2)	-19.70(1)
	3n	--	-9.24(1)	-18.66(0)
	3o	56.34(2)	1.02(2)	-14.66(2)
	3p	71.78(2)	13.62(2)	12.87(3)
$X_3H_6^+$	4a	0.0(1)	0.0(3)	0.0(3)
	4b	-40.68(0)	-58.79(0)	-60.47(0)
	4c	--	-73.69(0)	-85.79(0)
	4d	--	-59.92(1)	--
	4e	-22.09(2)	-57.54(1)	-68.56(0)
	4f	--	-67.99(0)	-72.58(0)
	4g	-1.11(2)	-46.93(1)	-63.58(1)
	4h	-32.50(0)	-45.83(1)	-52.41(2)
	4i	-23.96(1)	-42.51(2)	-48.81(3)
	4j	33.96(3)	-18.54(3)	-38.80(3)
	4k	188.25(4)	48.69(5)	-11.64(3)

^a Relative energies are calculated after scaling the zero point energy by 0.9806 (Scott, A.P.; Radom, L. *J. Phys. Chem.* **1996**, *100*, 16502).

^b C_3 symmetry.

Cartesian Coordinates

1a-B:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	5	0.000000	0.927918	0.000000
2	5	0.803601	-0.463959	0.000000
3	5	-0.803601	-0.463959	0.000000
4	1	0.000000	2.176879	0.000000
5	1	1.885232	-1.088439	0.000000
6	1	-1.885232	-1.088439	0.000000

1a-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	0.000000	1.450249	0.000000
2	13	1.255952	-0.725124	0.000000
3	13	-1.255952	-0.725124	0.000000
4	1	0.000000	3.129723	0.000000
5	1	2.710420	-1.564861	0.000000
6	1	-2.710420	-1.564861	0.000000

1a-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	1.429545	.000000
2	31	0	1.238023	-.714773	.000000
3	31	0	-1.238023	-.714773	.000000
4	1	0	.000000	3.115536	.000000
5	1	0	2.698134	-1.557768	.000000
6	1	0	-2.698134	-1.557768	.000000

1b-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	0.000000	1.434775	0.000000
2	31	0	-1.242551	-0.717387	0.000000
3	31	0	1.242551	-0.717387	0.000000
4	1	0	-0.351922	3.082275	0.000000
5	1	0	-2.493367	-1.845911	0.000000
6	1	0	2.845289	-1.236364	0.000000

1c-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	.885859
2	5	0	.000000	.851745	-.610217
3	5	0	.000000	-.851745	-.610217
4	1	0	.000000	.000000	-1.591697
5	1	0	.000000	.980152	1.632285
6	1	0	.000000	-.980152	1.632285

1c-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.435687
2	13	0	.000000	1.398288	-.834187
3	13	0	.000000	-1.398288	-.834187
4	1	0	.000000	.000000	-1.891880
5	1	0	.000000	1.297061	2.458407
6	1	0	.000000	-1.297061	2.458407

1c-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.431932
2	31	0	.000000	1.441291	-.765226
3	31	0	.000000	-1.441291	-.765226
4	1	0	.000000	.000000	-1.856802
5	1	0	.000000	1.286606	2.455468
6	1	0	.000000	-1.286606	2.455468

1d-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.978785	.000000
2	5	0	.847653	-.489393	.000000
3	5	0	-.847653	-.489393	.000000
4	1	0	.000000	-1.560830	.000000
5	1	0	-1.351719	.780415	.000000
6	1	0	1.351719	.780415	.000000

1d-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.680962	.970504	.000000
2	13	0	-1.680962	.970504	.000000
3	13	0	.000000	-1.941008	.000000
4	1	0	.000000	1.454458	.000000
5	1	0	-1.259598	-.727229	.000000
6	1	0	1.259598	-.727229	.000000

1d-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	-1.958842	.000000
2	31	0	1.696407	.979421	.000000
3	31	0	-1.696407	.979421	.000000
4	1	0	.000000	1.495295	.000000
5	1	0	-1.294964	-.747648	.000000
6	1	0	1.294964	-.747648	.000000

1e-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.998163	-.064349
2	5	0	.864435	-.499082	-.064349
3	5	0	-.864435	-.499082	-.064349
4	1	0	.000000	-1.475644	.321743
5	1	0	-1.277946	.737822	.321743
6	1	0	1.277946	.737822	.321743

1e-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	1.662675	-.060943
2	13	0	-1.439919	-.831338	-.060943
3	13	0	1.439919	-.831338	-.060943
4	1	0	-1.301191	.751243	.792262
5	1	0	.000000	-1.502487	.792262
6	1	0	1.301191	.751243	.792262

1e-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	31	0	.000000	1.714161	-.026403	
2	31	0	-1.484507	-.857081	-.026403	
3	31	0	1.484507	-.857081	-.026403	
4	1	0	-1.343794	.775840	.818487	
5	1	0	.000000	-1.551679	.818487	
6	1	0	1.343794	.775840	.818487	

1f-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	5	0	.000000	.827613	-.254861	
2	5	0	.000000	-.827613	-.254861	
3	5	0	.000000	.000000	1.151146	
4	1	0	.000000	.000000	-1.391919	
5	1	0	.000000	1.886022	-.907601	
6	1	0	.000000	-1.886022	-.907601	

1f-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	13	0	.000000	.000000	1.655696	
2	13	0	.000000	1.280603	-.622070	
3	13	0	.000000	-1.280603	-.622070	
4	1	0	.000000	.000000	-1.889395	
5	1	0	.000000	2.531035	-1.730412	
6	1	0	.000000	-2.531035	-1.730412	

1f-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.549060
2	31	0	.000000	1.322594	-.682675
3	31	0	.000000	-1.322594	-.682675
4	1	0	.000000	.000000	-1.983488
5	1	0	.000000	2.520772	-1.855770
6	1	0	.000000	-2.520772	-1.855770

1g-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.621406	-.695839	.000000
2	13	0	.000000	1.373980	.000000
3	13	0	-1.395970	-.639409	.000000
4	1	0	.016351	-1.644003	.000000
5	1	0	-.394421	2.973337	.000000
6	1	0	-2.552599	-1.832852	.000000

1g-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	1.587841	-.704616	.000000
2	31	0	.000000	1.327411	.000000
3	31	0	-1.481988	-.602348	.000000
4	1	0	-.070866	-1.674302	.000000
5	1	0	-.596328	2.857450	.000000
6	1	0	-2.614231	-1.817008	.000000

1h-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	.912980
2	5	0	.000000	.785341	-.629997
3	5	0	.000000	-.785341	-.629997
4	1	0	.000000	.000000	-1.624201
5	1	0	-1.003616	.000000	1.679636
6	1	0	1.003616	.000000	1.679636

1h-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.438719
2	13	0	.000000	1.383271	-.841708
3	13	0	.000000	-1.383271	-.841708
4	1	0	.000000	.000000	-1.863457
5	1	0	-1.262106	.000000	2.522255
6	1	0	1.262106	.000000	2.522255

1h-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.355462
2	31	0	.000000	1.666816	-.725246
3	31	0	.000000	-1.666816	-.725246
4	1	0	.000000	.000000	-1.749273
5	1	0	-1.317782	.000000	2.347598
6	1	0	1.317782	.000000	2.347598

1i-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-.324685	1.355403	.031790
2	13	0	1.663760	-.601602	-.065851
3	13	0	-1.444983	-.957635	-.031269
4	1	0	1.293986	1.050869	.610722
5	1	0	.200700	-1.341152	.655798
6	1	0	-.117883	2.940127	-.417226

1i-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-.463153	1.347861	.013374
2	31	0	1.795659	-.423740	-.025612
3	31	0	-1.370093	-1.015282	-.012454
4	1	0	1.218083	1.244226	.583547
5	1	0	.356820	-1.369221	.590266
6	1	0	-.409704	2.951001	-.408374

1j-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	.905802
2	5	0	.000000	.972698	-.451486
3	5	0	.000000	-.972698	-.451486
4	1	0	.818126	.000000	-1.075952
5	1	0	-.818126	.000000	-1.075952
6	1	0	.000000	.000000	2.137751

1j-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.491148
2	13	0	.000000	1.483436	-.784242
3	13	0	.000000	-1.483436	-.784242
4	1	0	1.081886	.000000	-1.079358
5	1	0	-1.081886	.000000	-1.079358
6	1	0	.000000	.000000	3.164082

1j-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.465026
2	31	0	.000000	1.536626	-.747387
3	31	0	.000000	-1.536626	-.747387
4	1	0	1.101679	.000000	-1.114389
5	1	0	-1.101679	.000000	-1.114389
6	1	0	.000000	.000000	3.150945

1k-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.851708	-.672552
2	5	0	.000000	-.851708	-.672552
3	5	0	.000000	.000000	.761420
4	1	0	.000000	.000000	1.987527
5	1	0	.000000	1.453443	.465447
6	1	0	.000000	-1.453443	.465447

1k-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	1.403976	-.831439
2	13	0	.000000	-1.403976	-.831439
3	13	0	.000000	.000000	1.292416
4	1	0	.000000	.000000	2.929052
5	1	0	.000000	1.800932	.943473
6	1	0	.000000	-1.800932	.943473

1k-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	1.420342	-.765640
2	31	0	.000000	-1.420342	-.765640
3	31	0	.000000	.000000	1.370405
4	1	0	.000000	.000000	3.001711
5	1	0	.000000	1.944189	.992714
6	1	0	.000000	-1.944189	.992714

2a-B:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	5	0.000000	0.853766	-0.356191
2	5	0.000000	-0.853766	-0.356191
3	5	0.000000	0.000000	0.954596
4	1	0.000000	0.000000	-1.366345
5	1	0.000000	1.877379	-0.997463
6	1	0.000000	-1.877379	-0.997463
7	1	0.000000	0.000000	2.150198

2a-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	0.000000	1.364573	-0.613747
2	13	0.000000	-1.364573	-0.613747
3	13	0.000000	0.000000	1.384131
4	1	0.000000	0.000000	-1.698769
5	1	0.000000	2.600680	-1.661013
6	1	0.000000	-2.600680	-1.661013
7	1	0.000000	0.000000	2.984521

2a-Ga:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	31	0.000000	1.398199	-0.608600
2	31	0.000000	-1.398199	-0.608600
3	31	0.000000	0.000000	1.287127
4	1	0.000000	0.000000	-1.722255
5	1	0.000000	2.614655	-1.652758
6	1	0.000000	-2.614655	-1.652758
7	1	0.000000	0.000000	2.860029

2b-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	-0.014322	-0.639349	1.323451
2	13	-0.014322	-0.639349	-1.323451
3	13	0.000000	1.432351	0.000000
4	1	0.764353	-1.510372	0.000000
5	1	0.167971	-1.679434	2.558608
6	1	0.167971	-1.679434	-2.558608
7	1	-0.727926	2.871758	0.000000

2b-Ga:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	31	-0.008890	-0.644912	1.351695
2	31	-0.008890	-0.644912	-1.351695
3	31	0.000000	1.360563	0.000000
4	1	0.822943	-1.532077	0.000000
5	1	0.317622	-1.669528	2.561244
6	1	0.317622	-1.669528	-2.561244
7	1	-0.907033	2.678186	0.000000

2c-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.622751
2	31	0	.000000	1.738158	-.876616
3	31	0	.000000	-1.738158	-.876616
4	1	0	.000000	.000000	-1.125551
5	1	0	.000000	1.472084	.983392
6	1	0	.000000	-1.472084	.983392
7	1	0	.000000	.000000	3.203686

2d-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-.057136	1.342059	.000000
2	13	0	-.057136	-.805581	1.551710
3	13	0	-.057136	-.805581	-1.551710
4	1	0	.765715	-1.210830	.000000
5	1	0	.857910	.883321	1.373029
6	1	0	.857910	.883321	-1.373029
7	1	0	-.253231	2.942534	.000000

2d-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-.026215	1.392877	.000000
2	31	0	-.026215	-.754949	1.583229
3	31	0	-.026215	-.754949	-1.583229
4	1	0	.743368	-1.328456	.000000
5	1	0	.957952	.986449	1.361723
6	1	0	.957952	.986449	-1.361723
7	1	0	-.221259	2.983209	.000000

2e-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.732669	-.638164
2	5	0	.000000	.000000	.925368
3	5	0	.000000	-.732669	-.638164
4	1	0	.000000	1.917038	-.725754
5	1	0	.000000	-1.917038	-.725754
6	1	0	.000000	.994264	1.603152
7	1	0	.000000	-.994264	1.603152

2e-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	1.122871	-.903952
2	13	0	.000000	.000000	1.546098
3	13	0	.000000	-1.122871	-.903952
4	1	0	.000000	2.703090	-.781686
5	1	0	.000000	-2.703090	-.781686
6	1	0	.000000	1.321376	2.483424
7	1	0	.000000	-1.321376	2.483424

2e-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	31	0	.000000	1.095792	-.836909	
2	31	0	.000000	.000000	1.559042	
3	31	0	.000000	-1.095792	-.836909	
4	1	0	.000000	2.641836	-.728329	
5	1	0	.000000	-2.641836	-.728329	
6	1	0	.000000	1.295479	2.507343	
7	1	0	.000000	-1.295479	2.507343	

2f-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	5	0	.000000	.000000	.896249	
2	5	0	.000000	.844735	-.533815	
3	5	0	.000000	-.844735	-.533815	
4	1	0	.000000	1.871047	-1.173135	
5	1	0	.000000	-1.871047	-1.173135	
6	1	0	-1.006918	.000000	1.601589	
7	1	0	1.006918	.000000	1.601589	

2f-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	13	0	.000000	.000000	1.507866	
2	13	0	.000000	1.314866	-.808358	
3	13	0	.000000	-1.314866	-.808358	
4	1	0	.000000	2.691280	-1.710638	
5	1	0	.000000	-2.691280	-1.710638	
6	1	0	-1.353332	.000000	2.418166	
7	1	0	1.353332	.000000	2.418166	

2f-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.481152
2	31	0	.000000	1.302195	-.764352
3	31	0	.000000	-1.302195	-.764352
4	1	0	.000000	2.684874	-1.661930
5	1	0	.000000	-2.684874	-1.661930
6	1	0	-1.329537	.000000	2.398982
7	1	0	1.329537	.000000	2.398982

2g-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	1.203097	-.902494
2	13	0	.000000	.000000	1.557901
3	13	0	.000000	-1.203097	-.902494
4	1	0	-1.222497	2.277263	-.906132
5	1	0	1.222497	-2.277263	-.906132
6	1	0	-1.022001	.827025	2.512198
7	1	0	1.022001	-.827025	2.512198

2g-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	1.177720	-.846942
2	31	0	.000000	.000000	1.581084
3	31	0	.000000	-1.177720	-.846942
4	1	0	-1.234207	2.225586	-.803333
5	1	0	1.234207	-2.225586	-.803333
6	1	0	-.890727	.935835	2.551737
7	1	0	.890727	-.935835	2.551737

2h-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	1.139181
2	5	0	.000000	.805296	-.379339
3	5	0	.000000	-.805296	-.379339
4	1	0	.000000	1.593646	.531405
5	1	0	.000000	-1.593646	.531405
6	1	0	.000000	1.276914	-1.482664
7	1	0	.000000	-1.276914	-1.482664

2h-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.649444
2	13	0	.000000	1.243702	-.711873
3	13	0	.000000	-1.243702	-.711873
4	1	0	.000000	2.150984	.634074
5	1	0	.000000	-2.150984	.634074
6	1	0	.000000	2.059560	-2.101107
7	1	0	.000000	-2.059560	-2.101107

2h-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.622536
2	31	0	.000000	1.200982	-.757990
3	31	0	.000000	-1.200982	-.757990
4	1	0	.000000	2.187664	.510893
5	1	0	.000000	-2.187664	.510893
6	1	0	.000000	1.942536	-2.162513
7	1	0	.000000	-1.942536	-2.162513

2i-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.254592	1.356357	-0.059500
2	13	0	-1.338951	-0.793892	0.074207
3	13	0	1.698593	-0.588998	-0.066293
4	1	0	-0.400638	2.955829	-0.060718
5	1	0	-2.153274	-1.962653	-0.684655
6	1	0	1.024527	0.860437	0.962128
7	1	0	0.163733	-1.508674	0.453852

2i-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-0.386051	1.302520	-0.046627
2	31	0	-1.327751	-0.887502	0.045767
3	31	0	1.767870	-0.420161	-0.022096
4	1	0	-0.870950	2.804415	0.186979
5	1	0	-1.963938	-2.066165	-0.845346
6	1	0	0.896998	0.977480	1.071617
7	1	0	0.261804	-1.556286	0.298389

2j-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	1.235799
2	5	0	.000000	.829840	-.249738
3	5	0	.000000	-.829840	-.249738
4	1	0	.898819	.000000	-.936799
5	1	0	-.898819	.000000	-.936799
6	1	0	.000000	1.848130	-.904006
7	1	0	.000000	-1.848130	-.904006

2j-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.807968
2	13	0	.000000	1.261285	-.661872
3	13	0	.000000	-1.261285	-.661872
4	1	0	1.108511	.000000	-1.303885
5	1	0	-1.108511	.000000	-1.303885
6	1	0	.000000	2.387329	-1.843567
7	1	0	.000000	-2.387329	-1.843567

2j-Ga:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	31	0.000000	0.000000	1.674055
2	31	0.000000	-1.309938	-0.728442
3	31	0.000000	1.309938	-0.728442
4	1	-1.129930	0.000000	-1.379647
5	1	1.129930	0.000000	-1.379647
6	1	0.000000	-2.343155	-1.986494
7	1	0.000000	2.343155	-1.986494

2k-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.043605	1.688499	0.000000
2	13	0	0.043605	-0.633451	1.278820
3	13	0	0.043605	-0.633451	-1.278820
4	1	0	-1.245593	-0.244210	0.000000
5	1	0	0.319997	-1.854755	0.000000
6	1	0	-0.387491	-1.690902	2.445385
7	1	0	-0.387491	-1.690902	-2.445385

2k-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-0.020657	1.591604	0.000000
2	31	0	-0.020657	-0.700373	1.336367
3	31	0	-0.020657	-0.700373	-1.336367
4	1	0	-0.351441	-1.917773	0.000000
5	1	0	1.321474	-0.314276	0.000000
6	1	0	0.475553	-1.842284	2.389744
7	1	0	0.475553	-1.842284	-2.389744

2l-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.938254	-.064456
2	5	0	.812552	-.469127	-.064456
3	5	0	-.812552	-.469127	-.064456
4	1	0	.000000	2.149226	-.039186
5	1	0	1.861284	-1.074613	-.039186
6	1	0	-1.861284	-1.074613	-.039186
7	1	0	.000000	.000000	1.084394

2l-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	0.000000	1.449841	-0.060557
2	13	1.255599	-0.724920	-0.060557
3	13	-1.255599	-0.724920	-0.060557
4	1	0.000000	3.034363	0.369611
5	1	2.627835	-1.517182	0.369611
6	1	-2.627835	-1.517182	0.369611
7	1	0.000000	0.000000	1.252871

2l-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	1.453760	-.027775
2	31	0	1.258993	-.726880	-.027775
3	31	0	-1.258993	-.726880	-.027775
4	1	0	.475117	2.964836	.404610
5	1	0	2.330065	-1.893882	.404610
6	1	0	-2.805182	-1.070954	.404610
7	1	0	.000000	.000000	1.369207

3a-B:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	5	0.000000	0.804627	-0.477055
2	5	0.000000	-0.804627	-0.477055
3	5	0.000000	0.000000	0.880884
4	1	0.000000	0.000000	2.060674
5	1	0.000000	1.493772	-1.429692
6	1	0.000000	-1.493772	-1.429692
7	1	0.000000	1.430362	0.582419
8	1	0.000000	-1.430362	0.582419

3a-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	0.000000	1.203288	-0.797799
2	13	0.000000	-1.203288	-0.797799
3	13	0.000000	0.000000	1.461940
4	1	0.000000	0.000000	3.027736
5	1	0.000000	2.595724	-1.522994
6	1	0.000000	-2.595724	-1.522994
7	1	0.000000	1.560818	0.877904
8	1	0.000000	-1.560818	0.877904

3a-Ga:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	31	0.000000	1.146423	-0.840648
2	31	0.000000	-1.146423	-0.840648
3	31	0.000000	0.000000	1.606612
4	1	0.000000	0.000000	3.153867
5	1	0.000000	2.609557	-1.333988
6	1	0.000000	-2.609557	-1.333988
7	1	0.000000	1.472673	0.914655
8	1	0.000000	-1.472673	0.914655

3b-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	-0.042660	-0.811240	1.208952
2	13	-0.042660	-0.811240	-1.208952
3	13	0.000000	1.478344	0.000000
4	1	0.396886	3.013632	0.000000
5	1	-0.573138	-1.191074	2.645274
6	1	-0.573138	-1.191074	-2.645274
7	1	0.929269	0.621141	1.260368
8	1	0.929269	0.621141	-1.260368

3b-Ga:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	31	-0.022463	-0.795508	1.180477
2	31	-0.022463	-0.795508	-1.180477
3	31	0.000000	1.533396	0.000000
4	1	0.592629	2.998850	0.000000
5	1	-0.602651	-1.190556	2.569845
6	1	-0.602651	-1.190556	-2.569845
7	1	1.002705	0.584254	1.304794
8	1	1.002705	0.584254	-1.304794

3c-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.000000	0.000000	1.767630
2	13	0	0.000000	1.819755	-1.076651
3	13	0	0.000000	-1.819755	-1.076651
4	1	0	0.000000	0.000000	-1.366133
5	1	0	0.000000	1.315386	0.692829
6	1	0	0.000000	-1.315386	0.692829
7	1	0	1.411330	0.000000	2.497106
8	1	0	-1.411330	0.000000	2.497106

3c-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.863289
2	31	0	.000000	1.827678	-1.018082
3	31	0	.000000	-1.827678	-1.018082
4	1	0	.000000	.000000	-1.401786
5	1	0	.000000	1.312764	.795844
6	1	0	.000000	-1.312764	.795844
7	1	0	1.395892	.000000	2.584603
8	1	0	-1.395892	.000000	2.584603

3d-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.010515	-1.480272	0.000000
2	13	0	1.774160	0.652382	0.000000
3	13	0	-1.804993	1.134907	0.000000
4	1	0	0.000000	1.215337	0.000000
5	1	0	0.921997	-0.702054	1.158282
6	1	0	-1.499231	-0.744859	0.000000
7	1	0	0.921997	-0.702054	-1.158282
8	1	0	-0.080630	-3.057600	0.000000

3d-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	0.038705	-1.586645	0.000000
2	31	0	1.774521	0.666534	0.000000
3	31	0	-1.821280	1.060215	0.000000
4	1	0	0.000000	1.312408	0.000000
5	1	0	0.885254	-0.823172	1.201071
6	1	0	-1.468120	-0.864229	0.000000
7	1	0	0.885254	-0.823172	-1.201071
8	1	0	-0.052719	-3.145071	0.000000

3e-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-0.012689	1.469873	0.000000
2	13	0	-0.012689	-0.881529	1.654571
3	13	0	-0.012689	-0.881529	-1.654571
4	1	0	0.696073	-1.161577	0.000000
5	1	0	0.703272	0.917294	1.390483
6	1	0	0.703272	0.917294	-1.390483
7	1	0	-1.099383	0.171559	0.000000
8	1	0	-0.508345	2.966834	0.000000

3f-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	2.073893
2	13	0	.000000	1.333501	-.887194
3	13	0	.000000	-1.333501	-.887194
4	1	0	.000000	.000000	-1.843101
5	1	0	.000000	1.206747	.702701
6	1	0	.000000	-1.206747	.702701
7	1	0	.000000	2.651615	-1.727927
8	1	0	.000000	-2.651615	-1.727927

3f-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	2.011127
2	31	0	.000000	1.328881	-.935226
3	31	0	.000000	-1.328881	-.935226
4	1	0	.000000	.000000	-1.918585
5	1	0	.000000	1.300779	.634095
6	1	0	.000000	-1.300779	.634095
7	1	0	.000000	2.566916	-1.855268
8	1	0	.000000	-2.566916	-1.855268

3g-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.050222	1.822251	.000000
2	13	0	.050222	-.771326	1.215491
3	13	0	.050222	-.771326	-1.215491
4	1	0	-.906462	-1.653686	.000000
5	1	0	-.853027	.624293	1.292325
6	1	0	-.853027	.624293	-1.292325
7	1	0	.326927	-1.614838	2.514758
8	1	0	.326927	-1.614838	-2.514758

3g-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.021812	1.785628	.000000
2	31	0	.021812	-.825055	1.201342
3	31	0	.021812	-.825055	-1.201342
4	1	0	-1.023694	-1.690540	.000000
5	1	0	-.893292	.513990	1.488315
6	1	0	-.893292	.513990	-1.488315
7	1	0	.390865	-1.769267	2.378576
8	1	0	.390865	-1.769267	-2.378576

3h-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.600567	-0.530224	0.000000
2	13	0	0.000000	1.377575	0.000000
3	13	0	1.688108	-0.918157	0.000000
4	1	0	0.915659	0.464187	1.114050
5	1	0	0.915659	0.464187	-1.114050
6	1	0	-2.915132	-1.417830	0.000000
7	1	0	-0.236798	-1.536252	0.000000
8	1	0	0.182574	2.946183	0.000000

3h-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-1.617937	-0.427329	0.000000
2	31	0	0.000000	1.378391	0.000000
3	31	0	1.663585	-0.990881	0.000000
4	1	0	0.930211	0.552491	1.156108
5	1	0	0.930211	0.552491	-1.156108
6	1	0	-2.981564	-1.211320	0.000000
7	1	0	-0.380188	-1.592750	0.000000
8	1	0	0.086226	2.933474	0.000000

3i-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.875139	-0.680764	0.000000
2	13	0	0.000000	1.394448	0.000000
3	13	0	1.428931	-0.755724	0.000000
4	1	0	1.117321	0.437399	1.145066
5	1	0	1.117321	0.437399	-1.145066
6	1	0	0.015689	-1.604393	0.000000
7	1	0	0.747785	2.802728	0.000000
8	1	0	2.802595	-1.526610	0.000000

3i-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-1.743712	-0.704286	0.000000
2	31	0	0.000000	1.433829	0.000000
3	31	0	1.537447	-0.741816	0.000000
4	1	0	1.227917	0.395862	1.186224
5	1	0	1.227917	0.395862	-1.186224
6	1	0	0.159306	-1.642081	0.000000
7	1	0	0.895110	2.751866	0.000000
8	1	0	2.883958	-1.521055	0.000000

3j-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	1.299264	-0.961429	0.000000
2	13	0	-1.521274	-0.874004	0.000000
3	13	0	0.000000	1.523139	0.000000
4	1	0	-0.785294	0.635302	1.163146
5	1	0	-0.785294	0.635302	-1.163146
6	1	0	2.887789	-1.203923	0.000000
7	1	0	1.566791	0.891684	0.000000
8	1	0	0.002135	3.101446	0.000000

3j-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	1.365270	-0.939893	0.000000
2	31	0	-1.460577	-0.856993	0.000000
3	31	0	0.000000	1.640889	0.000000
4	1	0	-0.771159	0.788581	1.194412
5	1	0	-0.771159	0.788581	-1.194412
6	1	0	2.979569	-0.980549	0.000000
7	1	0	1.555264	1.039773	0.000000
8	1	0	-0.037984	3.199542	0.000000

3k-B:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	5	0.000000	0.923314	0.000000
2	5	0.655190	-0.650500	0.000000
3	5	-0.965850	-0.402056	0.000000
4	1	0.208288	2.093796	0.000000
5	1	1.632426	-1.327603	0.000000
6	1	-2.055102	-0.855966	0.000000
7	1	0.883842	0.367990	0.884208
8	1	0.883842	0.367990	-0.884208

3k-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.181959	-.871009	.000000
2	13	0	.000000	1.468162	.000000
3	13	0	1.358406	-.686330	.000000
4	1	0	-2.661296	-1.455254	.000000
5	1	0	-.406832	3.005843	.000000
6	1	0	2.776905	-1.403316	.000000
7	1	0	-1.001292	.506013	1.110915
8	1	0	-1.001292	.506013	-1.110915

3k-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	1.344036	-.665916	.000000
2	31	0	-1.344033	-.665878	.000000
3	31	0	.000000	1.421628	.000000
4	1	0	2.507120	-1.729139	.000000
5	1	0	-2.507309	-1.728870	.000000
6	1	0	.000189	2.997672	.000000
7	1	0	-.000057	-1.162247	1.126832
8	1	0	-.000057	-1.162247	-1.126832

3I-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	5	0	.000000	.763794	-.487880	
2	5	0	.000000	.000000	.957927	
3	5	0	.000000	-.763794	-.487880	
4	1	0	.000000	1.904598	-.762941	
5	1	0	.000000	-1.904598	-.762941	
6	1	0	.000000	1.011006	1.576561	
7	1	0	.000000	-1.011006	1.576561	
8	1	0	.000000	.000000	-1.538072	

3I-AI:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	13	0	.000000	1.155760	-.753559	
2	13	0	.000000	.000000	1.498146	
3	13	0	.000000	-1.155760	-.753559	
4	1	0	.000000	2.677136	-1.095927	
5	1	0	.000000	-2.677136	-1.095927	
6	1	0	.000000	1.434295	2.170134	
7	1	0	.000000	-1.434295	2.170134	
8	1	0	.000000	.000000	-2.031777	

3I-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	31	0	.000000	1.140031	-.737636	
2	31	0	.000000	.000000	1.468947	
3	31	0	.000000	-1.140031	-.737636	
4	1	0	.000000	2.635073	-1.051885	
5	1	0	.000000	-2.635073	-1.051885	
6	1	0	.000000	1.381340	2.186332	
7	1	0	.000000	-1.381340	2.186332	
8	1	0	.000000	.000000	-2.072827	

3m-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	5	0	.000000	.000000	1.100541	
2	5	0	.000000	.729068	-.616057	
3	5	0	.000000	-.729068	-.616057	
4	1	0	.000000	.000000	-1.666063	
5	1	0	.000000	1.902950	-.544915	
6	1	0	.000000	-1.902950	-.544915	
7	1	0	1.026048	.000000	1.706878	
8	1	0	-1.026048	.000000	1.706878	

3m-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	13	0	0.000000	0.000000	1.468568	
2	13	0	0.000000	1.469302	-0.697148	
3	13	0	0.000000	-1.469302	-0.697148	
4	1	0	0.000000	0.000000	-1.768220	
5	1	0	0.000000	2.590435	-1.840058	
6	1	0	0.000000	-2.590435	-1.840058	
7	1	0	1.395468	0.000000	2.241394	
8	1	0	-1.395468	0.000000	2.241394	

3m-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms)		
				X	Y	Z
1	31	0	0.000000	0.000000	1.375259	
2	31	0	0.000000	1.500029	-0.669361	
3	31	0	0.000000	-1.500029	-0.669361	
4	1	0	0.000000	0.000000	-1.784206	
5	1	0	0.000000	2.603992	-1.817933	
6	1	0	0.000000	-2.603992	-1.817933	
7	1	0	1.371908	0.000000	2.143709	
8	1	0	-1.371908	0.000000	2.143709	

3n-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	0.000000	1.301543	-0.755456
2	13	0.000000	0.000000	1.516905
3	13	0.000000	-1.301543	-0.755456
4	1	-1.126632	2.258853	-1.347286
5	1	1.126632	-2.258853	-1.347286
6	1	-1.167680	0.767700	2.271841
7	1	1.167680	-0.767700	2.271841
8	1	0.000000	0.000000	-1.927006

3n-Ga:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	31	0.000000	1.317316	-0.724516
2	31	0.000000	0.000000	1.456712
3	31	0.000000	-1.317316	-0.724516
4	1	-1.069979	2.296707	-1.362128
5	1	1.069979	-2.296707	-1.362128
6	1	-1.165565	0.722369	2.213440
7	1	1.165565	-0.722369	2.213440
8	1	0.000000	0.000000	-1.940732

3o-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	.940476
2	5	0	.000000	.794998	-.574807
3	5	0	.000000	-.794998	-.574807
4	1	0	.000000	.000000	2.127082
5	1	0	1.011116	1.421453	-.270347
6	1	0	-1.011116	1.421453	-.270347
7	1	0	1.011116	-1.421453	-.270347
8	1	0	-1.011116	-1.421453	-.270347

3o-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.725622
2	13	0	.000000	1.251247	-.899555
3	13	0	.000000	-1.251247	-.899555
4	1	0	.000000	.000000	3.342165
5	1	0	1.346123	2.072700	-.596706
6	1	0	-1.346123	2.072700	-.596706
7	1	0	1.346123	-2.072700	-.596706
8	1	0	-1.346123	-2.072700	-.596706

3o-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.768123
2	31	0	.000000	1.213163	-.895926
3	31	0	.000000	-1.213163	-.895926
4	1	0	.000000	.000000	3.397486
5	1	0	1.333308	2.047770	-.665469
6	1	0	-1.333308	2.047770	-.665469
7	1	0	1.333308	-2.047770	-.665469
8	1	0	-1.333308	-2.047770	-.665469

3p-B:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	5	0.000000	0.990288	0.000000
2	5	0.857615	-0.495144	0.000000
3	5	-0.857615	-0.495144	0.000000
4	1	0.000000	2.175976	0.000000
5	1	1.884451	-1.087988	0.000000
6	1	-1.884451	-1.087988	0.000000
7	1	0.000000	0.000000	0.972148
8	1	0.000000	0.000000	-0.972148

3p-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	0.000000	1.494827	0.000000
2	13	1.294558	-0.747413	0.000000
3	13	-1.294558	-0.747413	0.000000
4	1	0.000000	3.089888	0.000000
5	1	2.675921	-1.544944	0.000000
6	1	-2.675921	-1.544944	0.000000
7	1	0.000000	0.000000	1.084132
8	1	0.000000	0.000000	-1.084132

3p-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	1.517204	.000000
2	31	0	1.313937	-.758602	.000000
3	31	0	-1.313937	-.758602	.000000
4	1	0	.000000	3.109547	.000000
5	1	0	2.692947	-1.554773	.000000
6	1	0	-2.692947	-1.554773	.000000
7	1	0	.000000	.000000	1.099414
8	1	0	.000000	.000000	-1.099414

4a-B:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	5	0.000000	0.937719	0.000000
2	5	0.812089	-0.468860	0.000000
3	5	-0.812089	-0.468860	0.000000
4	1	0.000000	2.118676	0.000000
5	1	1.834827	-1.059338	0.000000
6	1	-1.834827	-1.059338	0.000000
7	1	1.276704	0.737105	0.000000
8	1	0.000000	-1.474211	0.000000
9	1	-1.276704	0.737105	0.000000

4a-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	1.431554	0.826508	0.000000
2	13	-1.431554	0.826508	0.000000
3	13	0.000000	-1.653016	0.000000
4	1	2.772370	1.600629	0.000000
5	1	-2.772370	1.600629	0.000000
6	1	0.000000	-3.201257	0.000000
7	1	0.000000	1.566925	0.000000
8	1	-1.356997	-0.783463	0.000000
9	1	1.356997	-0.783463	0.000000

4a-Ga:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	31	.000000	1.613110	.000000
2	31	1.396994	-.806555	.000000
3	31	-1.396994	-.806555	.000000
4	1	.000000	3.139918	.000000
5	1	2.719249	-1.569959	.000000
6	1	-2.719249	-1.569959	.000000
7	1	1.422238	.821129	.000000
8	1	.000000	-1.642259	.000000
9	1	-1.422238	.821129	.000000

4b-B:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	5	0.000000	0.955200	-0.044875
2	5	0.827227	-0.477600	-0.044875
3	5	-0.827227	-0.477600	-0.044875
4	1	0.000000	2.069619	-0.411505
5	1	1.792343	-1.034809	-0.411505
6	1	-1.792343	-1.034809	-0.411505
7	1	1.110667	0.641244	0.635879
8	1	0.000000	-1.282487	0.635879
9	1	-1.110667	0.641244	0.635879

4b-Al:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	13	0.000000	1.473513	-0.040162
2	13	-1.276100	-0.736756	-0.040162
3	13	1.276100	-0.736756	-0.040162
4	1	0.000000	2.989538	-0.371002
5	1	-2.589016	-1.494769	-0.371002
6	1	2.589016	-1.494769	-0.371002
7	1	-1.267960	0.732057	0.893110
8	1	0.000000	-1.464114	0.893110
9	1	1.267960	0.732057	0.893110

4b-Ga:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	31	0.000000	1.456104	-0.020324
2	31	-1.261023	-0.728052	-0.020324
3	31	1.261023	-0.728052	-0.020324
4	1	0.000000	2.953081	-0.335963
5	1	-2.557443	-1.476541	-0.335963
6	1	2.557443	-1.476541	-0.335963
7	1	-1.285825	0.742371	0.965992
8	1	0.000000	-1.484742	0.965992
9	1	1.285825	0.742371	0.965992

4c-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.452885	0.709164	0.000000
2	13	0	-0.291207	-1.590062	0.000000
3	13	0	2.090338	1.055819	0.000000
4	1	0	1.177473	-0.868182	0.000000
5	1	0	-1.078627	-0.544803	1.139588
6	1	0	0.000000	1.462250	0.000000
7	1	0	-1.078627	-0.544803	-1.139588
8	1	0	-2.879846	1.326283	0.000000
9	1	0	-0.641563	-3.104708	0.000000

4c-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	1.046464	1.295573	0.000006
2	31	0	1.046684	-1.295489	-0.000001
3	31	0	-2.274811	-0.000094	-0.000006
4	1	0	-0.560459	-1.406015	-0.000005
5	1	0	1.261014	0.000086	-1.176504
6	1	0	-0.560732	1.405760	0.000002
7	1	0	1.261007	0.000081	1.176510
8	1	0	2.115088	2.396855	0.000011
9	1	0	2.115651	-2.396438	0.000000

4d-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	0.000000	1.530067	0.000000
2	13	0	-1.982868	-0.674797	0.000000
3	13	0	1.691377	-0.992751	0.000000
4	1	0	0.222311	-1.603228	0.000000
5	1	0	-0.752938	0.645534	1.170164
6	1	0	1.569174	0.653562	0.000000
7	1	0	-0.752938	0.645534	-1.170164
8	1	0	0.379993	3.042454	0.000000
9	1	0	3.123790	-1.596601	0.000000

4e-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	.909267
2	5	0	.000000	.888628	-.537770
3	5	0	.000000	-.888628	-.537770
4	1	0	-1.032168	.000000	1.515336
5	1	0	1.032168	.000000	1.515336
6	1	0	.000000	1.435941	-1.576395
7	1	0	.000000	-1.435941	-1.576395
8	1	0	.000000	1.559481	.476738
9	1	0	.000000	-1.559481	.476738

4e-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.886051
2	13	0	.000000	1.284464	-1.047053
3	13	0	.000000	-1.284464	-1.047053
4	1	0	-1.475402	.000000	2.407763
5	1	0	1.475402	.000000	2.407763
6	1	0	.000000	2.701200	-1.702756
7	1	0	.000000	-2.701200	-1.702756
8	1	0	.000000	1.305946	.647358
9	1	0	.000000	-1.305946	.647358

4e-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.962883
2	31	0	.000000	1.243225	-1.027291
3	31	0	.000000	-1.243225	-1.027291
4	1	0	-1.470058	.000000	2.434606
5	1	0	1.470058	.000000	2.434606
6	1	0	.000000	2.641255	-1.690927
7	1	0	.000000	-2.641255	-1.690927
8	1	0	.000000	1.322213	.677643
9	1	0	.000000	-1.322213	.677643

4f-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	-1.596315	-0.562514	0.000000
2	13	0	0.000000	1.415922	0.000000
3	13	0	1.428340	-0.779546	0.000000
4	1	0	0.956251	0.407319	1.132890
5	1	0	0.956251	0.407319	-1.132890
6	1	0	-2.782427	-1.582875	0.000000
7	1	0	-0.074290	-1.566341	0.000000
8	1	0	0.353389	2.932990	0.000000
9	1	0	2.774506	-1.558617	0.000000

4f-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-1.574869	-0.533712	0.000000
2	31	0	0.000000	1.368470	0.000000
3	31	0	1.494225	-0.802330	0.000000
4	1	0	0.998660	0.396192	1.163611
5	1	0	0.998660	0.396192	-1.163611
6	1	0	-2.702599	-1.601669	0.000000
7	1	0	0.027909	-1.609831	0.000000
8	1	0	0.296742	2.877461	0.000000
9	1	0	2.880592	-1.463620	0.000000

4g-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	1.016973
2	5	0	.000000	.872778	-.468835
3	5	0	.000000	-.872778	-.468835
4	1	0	.000000	.000000	-1.456126
5	1	0	.000000	.000000	2.190868
6	1	0	1.043276	1.440037	-.282814
7	1	0	-1.043276	1.440037	-.282814
8	1	0	-1.043276	-1.440037	-.282814
9	1	0	1.043276	-1.440037	-.282814

4g-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.729281
2	13	0	.000000	1.453258	-.822441
3	13	0	.000000	-1.453258	-.822441
4	1	0	.000000	.000000	-1.697706
5	1	0	.000000	.000000	3.306100
6	1	0	1.455120	2.015292	-.676392
7	1	0	-1.455120	2.015292	-.676392
8	1	0	-1.455120	-2.015292	-.676392
9	1	0	1.455120	-2.015292	-.676392

4g-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.690509
2	31	0	.000000	1.471562	-.824672
3	31	0	.000000	-1.471562	-.824672
4	1	0	.000000	.000000	-1.708214
5	1	0	.000000	.000000	3.269557
6	1	0	1.452939	1.987824	-.709367
7	1	0	-1.452939	1.987824	-.709367
8	1	0	-1.452939	-1.987824	-.709367
9	1	0	1.452939	-1.987824	-.709367

4h-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	1.135206
2	5	0	.000000	.756797	-.538888
3	5	0	.000000	-.756797	-.538888
4	1	0	.932270	.000000	-1.131808
5	1	0	-.932270	.000000	-1.131808
6	1	0	.000000	1.019184	1.738271
7	1	0	.000000	-1.019184	1.738271
8	1	0	.000000	1.907111	-.750035
9	1	0	.000000	-1.907111	-.750035

4h-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.757149
2	13	0	.000000	1.156732	-.862342
3	13	0	.000000	-1.156732	-.862342
4	1	0	1.117812	.000000	-1.523348
5	1	0	-1.117812	.000000	-1.523348
6	1	0	.000000	1.423232	2.426022
7	1	0	.000000	-1.423232	2.426022
8	1	0	.000000	2.686553	-1.113695
9	1	0	.000000	-2.686553	-1.113695

4h-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.704036
2	31	0	.000000	1.147183	-.843835
3	31	0	.000000	-1.147183	-.843835
4	1	0	1.157792	.000000	-1.560585
5	1	0	-1.157792	.000000	-1.560585
6	1	0	.000000	1.393739	2.391945
7	1	0	.000000	-1.393739	2.391945
8	1	0	.000000	2.651662	-1.085044
9	1	0	.000000	-2.651662	-1.085044

4i-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.000000	1.218309
2	5	0	.000000	.737696	-.605043
3	5	0	.000000	-.737696	-.605043
4	1	0	.953537	.000000	-1.187110
5	1	0	-.953537	.000000	-1.187110
6	1	0	1.058141	.000000	1.739748
7	1	0	-1.058141	.000000	1.739748
8	1	0	.000000	1.910398	-.573197
9	1	0	.000000	-1.910398	-.573197

4i-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	.000000	1.818946
2	13	0	.000000	1.149193	-.898566
3	13	0	.000000	-1.149193	-.898566
4	1	0	1.124360	.000000	-1.556602
5	1	0	-1.124360	.000000	-1.556602
6	1	0	1.430492	.000000	2.463960
7	1	0	-1.430492	.000000	2.463960
8	1	0	.000000	2.694260	-1.049148
9	1	0	.000000	-2.694260	-1.049148

4i-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	.000000	1.795046
2	31	0	.000000	1.134966	-.888773
3	31	0	.000000	-1.134966	-.888773
4	1	0	1.164338	.000000	-1.614358
5	1	0	-1.164338	.000000	-1.614358
6	1	0	1.428703	.000000	2.401620
7	1	0	-1.428703	.000000	2.401620
8	1	0	.000000	2.650525	-1.058502
9	1	0	.000000	-2.650525	-1.058502

4j-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	1.159505	.000000
2	5	0	1.004161	-.579753	.000000
3	5	0	-1.004161	-.579753	.000000
4	1	0	.000000	1.622240	1.089266
5	1	0	.000000	1.622240	-1.089266
6	1	0	1.404901	-.811120	1.089266
7	1	0	1.404901	-.811120	-1.089266
8	1	0	-1.404901	-.811120	1.089266
9	1	0	-1.404901	-.811120	-1.089266

4j-Al:

Standard orientation:

Center Number	Atomic Number		Coordinates (Angstroms)		
			X	Y	Z
1	13	0.000000	1.716322	0.000000	
2	13	1.486379	-0.858161	0.000000	
3	13	-1.486379	-0.858161	0.000000	
4	1	0.000000	2.307850	1.453846	
5	1	0.000000	2.307850	-1.453846	
6	1	1.998657	-1.153925	1.453846	
7	1	1.998657	-1.153925	-1.453846	
8	1	-1.998657	-1.153925	1.453846	
9	1	-1.998657	-1.153925	-1.453846	

4j-Ga:

Standard orientation:

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	31	0.000000	1.678018	0.000000
2	31	1.453206	-0.839009	0.000000
3	31	-1.453206	-0.839009	0.000000
4	1	0.000000	2.244545	1.447219
5	1	0.000000	2.244545	-1.447219
6	1	1.943833	-1.122272	1.447219
7	1	1.943833	-1.122272	-1.447219
8	1	-1.943833	-1.122272	1.447219
9	1	-1.943833	-1.122272	-1.447219

4k-B:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	5	0	.000000	.893066	.000000
2	5	0	-.773417	-.446533	.000000
3	5	0	.773417	-.446533	.000000
4	1	0	.000000	-1.154331	.984728
5	1	0	.999680	.577166	.984728
6	1	0	-.999680	.577166	.984728
7	1	0	.000000	-1.154331	-.984728
8	1	0	.999680	.577166	-.984728
9	1	0	-.999680	.577166	-.984728

4k-Al:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	13	0	.000000	2.638864	.000000
2	13	0	-2.285324	-1.319432	.000000
3	13	0	2.285324	-1.319432	.000000
4	1	0	.000000	-1.311072	.407060
5	1	0	1.135422	.655536	.407060
6	1	0	-1.135422	.655536	.407060
7	1	0	.000000	-1.311072	-.407060
8	1	0	1.135422	.655536	-.407060
9	1	0	-1.135422	.655536	-.407060

4k-Ga:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	.000000	2.746763	.000000
2	31	0	-2.378767	-1.373382	.000000
3	31	0	2.378767	-1.373382	.000000
4	1	0	.000000	-1.403690	.396989
5	1	0	1.215631	.701845	.396989
6	1	0	-1.215631	.701845	.396989
7	1	0	.000000	-1.403690	-.396989
8	1	0	1.215631	.701845	-.396989
9	1	0	-1.215631	.701845	-.396989