

SUPPLEMENT 1 TABLE 1A: Aluminum models

Ring	Edge type	Ext rot (<i>E</i>)	Int rot (<i>I</i>)	$\sum_{\text{half}} E$	$\sum_{\text{half}} I$	Dist of <i>E</i> (α)	DAD (<i>D</i>)	Twist (<i>T</i>)	$\sum_{\text{half}} D$	$\sum_{\text{half}} D/2$	$\sum_{\text{half}} T$
611											
pent	Sym	0.00	0.00	-31.51	0.00		0.00	0.00	31.51	15.76	-15.76
hex	Green	-16.34	12.03			52%	28.37	-2.16			
hex	Twist	-15.17	-12.03			48%	3.14	-13.60			
hex	Sym	0.00	0.00	31.51	0.00		0.00	0.00	-31.51	-15.76	15.76
hex	Twist	15.17	12.03				-3.14	13.60			
hex	Green	16.34	-12.03				-28.37	2.16			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
621											
pent	Red	-8.65	8.37	-48.45	-3.78	18%	17.02	-0.14	44.67	22.34	-26.12
hex	Green	-21.98	3.76			45%	25.74	-9.11			
hex	Twist	-17.82	-15.91			37%	1.91	-16.87			
hex	Twist	17.82	15.91	48.45	3.78		-1.91	16.87	-44.67	-22.34	26.12
hex	Green	21.98	-3.76				-25.74	9.11			
pent	Red	8.65	-8.37				-17.02	0.14			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
622											
hex	Sym	0.00	0.00	-28.68	0.00		0.00	0.00	28.68	14.34	-14.34
pent	Twist	-10.73	-11.22			37%	-0.49	-10.98			
hex	Green	-17.95	11.22			63%	29.17	-3.37			
hex	Sym	0.00	0.00	28.68	0.00		0.00	0.00	-28.68	-14.34	14.34
hex	Green	17.95	-11.22				-29.17	3.37			
pent	Twist	10.73	11.22				0.49	10.98			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
623											
pent	Sym	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00	0.00
hex	Green	-12.90	14.55				27.45	0.83			
hex	Green	12.90	-14.55				-27.45	-0.83			
pent	Sym	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00	0.00
hex	Green	-12.90	14.55				27.45	0.83			
hex	Green	12.90	-14.55				-27.45	-0.83			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00

SUPPLEMENT 1 TABLE 1A: Aluminum models (continued)

Ring	Edge type	Ext rot (<i>E</i>)	Int rot (<i>I</i>)	$\sum_{\text{half}} E$	$\sum_{\text{half}} I$	Dist of <i>E</i> (α)	DAD (<i>D</i>)	Twist (<i>T</i>)	$\sum_{\text{half}} D$	$\sum_{\text{half}} D/2$	$\sum_{\text{half}} T$
631											
pent	Sym	0.00	0.00	-42.82	0.00		0.00	0.00	42.82	21.41	-21.41
pent	Red	-16.65	0.03			39%	16.68	-8.31			
hex	Green	-26.17	-0.03			61%	26.14	-13.10			
hex	Sym	0.00	0.00	42.82	0.00		0.00	0.00	-42.82	-21.41	21.41
hex	Green	26.17	0.03				-26.14	13.10			
pent	Red	16.65	-0.03				-16.68	8.31			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
632											
pent	Red	-14.94	3.57	-18.91	-0.11		18.51	-5.69	18.80	9.40	-9.51
hex	Green	-29.50	2.13				31.63	-13.69			
hex	Green	25.53	-5.81				-31.34	9.86			
pent	Twist	3.89	3.85	19.00	0.16		-0.04	3.87	-18.84	-9.42	0.07
hex	Twist	2.81	1.84				-0.97	2.33			
pent	Red	12.30	-5.53				-17.83	3.39			
	Sum			0.09	0.05		-0.04	0.07	-0.04	-0.02	-9.44
641											
hex	Green	-18.29	8.87	-43.14	0.40	42%	27.16	-4.71	43.54	21.77	-21.37
pent	Red	-17.58	-0.41			41%	17.17	-9.00			
pent	Twist	-7.27	-8.06			17%	-0.79	-7.67			
pent	Twist	7.27	8.06	43.14	-0.40		0.79	7.67	-43.54	-21.77	21.37
pent	Red	17.58	0.41				-17.17	9.00			
hex	Green	18.29	-8.87				-27.16	4.71			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
642											
hex	Sym	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00	0.00
pent	Red	3.60	-14.06				-17.66	-5.23			
pent	Red	-3.60	14.06				17.66	5.23			
hex	Sym	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00	0.00
pent	Red	3.60	-14.06				-17.66	-5.23			
pent	Red	-3.60	14.06				17.66	5.23			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00

SUPPLEMENT 1 TABLE 1A: Aluminum models (continued)

Ring	Edge type	Ext rot (<i>E</i>)	Int rot (<i>I</i>)	$\sum_{\text{half}} E$	$\sum_{\text{half}} I$	Dist of <i>E</i> (α)	DAD (<i>D</i>)	Twist (<i>T</i>)	$\sum_{\text{half}} D$	$\sum_{\text{half}} D/2$	$\sum_{\text{half}} T$
643											
pent	Sym	0.00	0.00	-18.20	0.00		0.00	0.00	18.20	9.10	-9.10
hex	Twist	-9.96	-9.42			55%	0.54	-9.69			
pent	Red	-8.24	9.42			45%	17.66	0.59			
pent	Sym	0.00	0.00	18.20	0.00		0.00	0.00	-18.20	-9.10	9.10
pent	Red	8.24	-9.42				-17.66	-0.59			
hex	Twist	9.96	9.42				-0.54	9.69			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
651											
hex	Sym	0.00	0.00	-18.01	0.00		0.00	0.00	18.01	9.01	-9.01
pent	Twist	-8.12	-8.40			45%	-0.28	-8.26			
pent	Red	-9.89	8.40			55%	18.29	-0.75			
pent	Sym	0.00	0.00	18.01	0.00		0.00	0.00	-18.01	-9.01	9.01
pent	Red	9.89	-8.40				-18.29	0.75			
pent	Twist	8.12	8.40				0.28	8.26			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
511											
pent	Sym	0.00	0.00				0.00	0.00			
hex	Red	-12.60	5.09	-21.17	-3.15	60%	17.69	-3.76	18.02	9.01	-12.16
hex	Twist	-8.57	-8.24			40%	0.33	-8.41			
hex	Twist	8.57	8.24	21.17	3.15		-0.33	8.41			
hex	Red	12.60	-5.09				-17.69	3.76	-17.69	-8.85	3.76
	Sum			0.00	0.00		0.00	0.00	0.33	0.16	-8.41
521											
pent	BLUE	-10.88	3.03	-30.50	1.16	36%	13.91	-3.93	31.66	15.83	-14.67
hex	Red	-19.62	-1.87			64%	17.75	-10.75			
hex	Sym	0.00	0.00				0.00	0.00			
hex	Red	19.62	1.87	30.50	-1.16		-17.75	10.75	-31.66	-15.83	14.67
pent	BLUE	10.88	-3.03				-13.91	3.93			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
522											
pent	Twist	-5.98	-6.23	-14.09	3.52	42%	-0.25	-6.11	17.61	8.81	-5.29
hex	Red	-8.11	9.75			58%	17.86	0.82			
hex	Red	8.30	-9.55	14.10	-3.52		-17.85	-0.63	-17.62	-8.81	5.29
pent	Twist	5.44	5.71				0.27	5.58			
hex	Sym*	0.36	0.32				-0.04	0.34			
	Sum			0.01	0.00		0.03	-0.34	-0.01	-0.01	0.00

SUPPLEMENT 1 TABLE 1A: Aluminum models (continued)

Ring	Edge type	Ext rot (<i>E</i>)	Int rot (<i>I</i>)	$\sum_{\text{half}} E$	$\sum_{\text{half}} I$	Dist of <i>E</i> (α)	DAD (<i>D</i>)	Twist (<i>T</i>)	$\sum_{\text{half}} D$	$\sum_{\text{half}} D/2$	$\sum_{\text{half}} T$
531											
pent	Sym	0.00	0.00								
pent	BLUE	-15.05	-1.24	-31.01	0.76	49%	13.81	-8.15	31.77	15.89	-15.13
hex	Red	-15.96	2.00			51%	17.96	-6.98			
hex	Red	15.96	-2.00	31.01	-0.76		-17.96	6.98	-31.77	-15.89	15.13
pent	BLUE	15.05	1.24				-13.81	8.15			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
532											
hex	Twist	-5.99	-5.70	-11.20	3.52	53%	0.29	-5.85	14.72	7.36	-3.84
pent	BLUE	-5.21	9.22			47%	14.43	2.01			
pent	BLUE	5.21	-9.22	11.20	-3.52		-14.43	-2.01	-14.72	-7.36	3.84
hex	Twist	5.99	5.70				-0.29	5.85			
pent	Sym	0.00	0.00				0.00	0.00			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
541											
pent	Twist	-6.27	-6.52	-16.82	-2.49	37%	-0.25	-6.40	14.33	7.17	-9.66
pent	BLUE	-10.55	4.03			63%	14.58	-3.26			
hex	Sym	0.00	0.00				0.00	0.00			
pent	BLUE	10.55	-4.03	16.82	2.49		-14.58	3.26	-14.33	-7.17	9.66
pent	Twist	6.27	6.52				0.25	6.40			
	Sum			0.00	0.00		0.00	0.00	0.25	0.00	0.00

Supplement 1 Table 1A. Angles of interest (in degrees) associated with all of the edges of all the hex-Rings and pent-Rings composed of aluminum atoms.

Edge lengths were constrained to 2.5 Å. Internal angles were constrained to 108° in pentagonal faces and 120° in hexagonal faces. Electrostatic interactions were turned off. The equilibrium geometry of each Ring structure was determined by molecular mechanics calculations (MMFF94) (20-24) in Spartan '04. External rotation (*E*) and internal rotation (*I*) were measured. DAD (*D*) and twist (*T*) were calculated from *E* and *I* according to Eqs. 1 and 2.

SUPPLEMENT 1 TABLE 1B: Carbon models

Ring	Edge type	Ext rot (E)	Int rot (I)	$\sum_{\text{half}} E$	$\sum_{\text{half}} I$	Dist of E (α)	DAD (D)	Twist (T)	$\sum_{\text{half}} D$	$\sum_{\text{half}} D/2$	$\sum_{\text{half}} T$
611											
pent	Sym	0.00	0.00	-32.19	0.02		0.00	0.00	32.21	16.11	-
16.09											
hex	Green	-18.27	10.00			57%	28.27	-4.14			
hex	Twist	-13.92	-9.98			43%	3.94	-11.95			
hex	Sym	0.00	0.00	32.19	-0.02		0.00	0.00	-32.21	-16.11	16.09
hex	Twist	13.92	9.98				-3.94	11.95			
hex	Green	18.27	-10.00				-28.27	4.14			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
621											
pent	Red	-13.58	3.99	-51.23	-4.32	27%	17.57	-4.80	46.91	23.46	-27.78
hex	Green	-22.50	4.31			44%	26.81	-9.10			
hex	Twist	-15.15	-12.62			30%	2.53	-13.89			
hex	Twist	15.15	12.62	51.23	4.32		-2.53	13.89	-46.91	-23.46	27.78
hex	Green	22.50	-4.31				-26.81	9.10			
pent	Red	13.58	-3.99				-17.57	4.80			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
622											
hex	Sym	0.00	0.00	-27.83	-0.01		0.00	0.00	27.82	13.91	-13.92
pent	Twist	-8.50	-8.74			31%	-0.24	-8.62			
hex	Green	-19.33	8.73			69%	28.06	-5.30			
hex	Sym	0.00	0.00	27.83	0.01		0.00	0.00	-27.82	-13.91	13.92
hex	Green	19.33	-8.73				-28.06	5.30			
pent	Twist	8.50	8.74				0.24	8.62			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
623											
pent	Sym	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00	0.00
hex	Green	-12.74	13.78				26.52	0.52			
hex	Green	12.74	-13.78				-26.52	-0.52			
pent	Sym	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00	0.00
hex	Green	-12.74	13.78				26.52	0.52			
hex	Green	12.74	-13.78				-26.52	-0.52			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00

SUPPLEMENT 1 TABLE 1B: Carbon models (continued)

Ring	Edge type	Ext rot (<i>E</i>)	Int rot (<i>I</i>)	$\sum_{\text{half}} E$	$\sum_{\text{half}} I$	Dist of <i>E</i> (α)	DAD (<i>D</i>)	Twist (<i>T</i>)	$\sum_{\text{half}} D$	$\sum_{\text{half}} D/2$	$\sum_{\text{half}} T$
631											
pent	Sym	0.00	0.00	-43.84	-0.01		0.00	0.00	43.83	21.92	-21.93
pent	Red	-18.91	-2.37			43%	16.54	-10.64			
hex	Green	-24.93	2.36			57%	27.29	-11.29			
hex	Sym	0.00	0.00	43.84	0.01		0.00	0.00	-43.83	-21.92	21.93
hex	Green	24.93	-2.36				-27.29	11.29			
pent	Red	18.91	2.37				-16.54	10.64			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
632											
pent	Red	-12.51	5.05	-19.71	-1.37		17.56	-3.73	18.34	9.17	-10.54
hex	Green	-17.12	9.69				26.81	-3.72			
hex	Green	9.92	-16.11				-26.03	-3.10			
pent	Twist	8.00	7.72	19.63	1.31		-0.28	7.86	-18.32	-9.16	-0.07
hex	Twist	6.80	7.05				0.25	6.93			
pent	Red	4.83	-13.46				-18.29	-4.32			
	Sum			-0.08	-0.06		0.02	-0.07	0.02	0.01	-10.61
641											
hex	Green	-13.16	15.45	-44.25	1.24	30%	28.61	1.15	45.49	22.75	-21.51
pent	Red	-18.93	-1.27			43%	17.66	-10.10			
pent	Twist	-12.16	-12.94			27%	-0.78	-12.55			
pent	Twist	12.16	12.94	44.25	-1.24		0.78	12.55	-45.49	-22.75	21.51
pent	Red	18.93	1.27				-17.66	10.10			
hex	Green	13.16	-15.45				-28.61	-1.15			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
642											
hex	Sym	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00	0.00
pent	Red	6.89	-10.95				-17.84	-2.03			
pent	Red	-6.89	10.95				17.84	2.03			
hex	Sym	0.00	0.00	0.00	0.00		0.00	0.00	0.00	0.00	0.00
pent	Red	6.89	-10.95				-17.84	-2.03			
pent	Red	-6.89	10.95				17.84	2.03			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00

SUPPLEMENT 1 TABLE 1B: Carbon models (continued)

Ring	Edge type	Ext rot (<i>E</i>)	Int rot (<i>I</i>)	$\sum_{\text{half}} E$	$\sum_{\text{half}} I$	Dist of <i>E</i> (α)	DAD (<i>D</i>)	Twist (<i>T</i>)	$\sum_{\text{half}} D$	$\sum_{\text{half}} D/2$	$\sum_{\text{half}} T$
643											
pent	Sym	0.00	0.00	-18.64	-0.01		0.00	0.00	18.63	9.32	-9.33
hex	Twist	-9.29	-8.70			50%	0.59	-9.00			
pent	Red	-9.35	8.69			50%	18.04	-0.33			
pent	Sym	0.00	0.00	18.64	0.01		0.00	0.00	-18.63	-9.32	9.33
pent	Red	9.35	-8.69				-18.04	0.33			
hex	Twist	9.29	8.70				-0.59	9.00			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
651											
hex	Sym	-0.03	-0.04	-18.36	0.04		-0.01	-0.04	18.40	9.20	-9.16
pent	Twist	-8.55	-8.91			47%	-0.36	-8.73			
pent	Red	-9.78	8.99			53%	18.77	-0.40			
pent	Sym	-0.10	-0.12	18.38	-0.04		-0.02	-0.11	-18.42	-9.21	9.17
pent	Red	9.94	-8.83				-18.77	0.56			
pent	Twist	8.54	8.91				0.37	8.73			
	Sum			0.02	0.00		-0.02	0.01	-0.02	-0.01	0.01
511											
pent	Sym	0.00	0.00				0.00	0.00			
hex	Red	-14.93	2.60	-19.57	-1.61	76%	17.53	-6.17	17.96	8.98	-10.59
hex	Twist	-4.64	-4.21			24%	0.43	-4.43			
hex	Twist	4.64	4.21	19.57	1.61		-0.43	4.43			
hex	Red	14.93	-2.60				-17.53	6.17	-17.53	-8.77	6.17
	Sum			0.00	0.00		0.00	0.00	0.43	0.22	-4.43
521											
pent	BLUE	-14.93	-0.89	-32.64	-0.34	46%	14.04	-7.91	32.30	16.15	-16.49
hex	Red	-17.71	0.55			54%	18.26	-8.58			
hex	Sym	0.00	0.00				0.00	0.00			
hex	Red	17.71	-0.55	32.64	0.34		-18.26	8.58	-32.30	-16.15	16.49
pent	BLUE	14.93	0.89				-14.04	7.91			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
522											
pent	Twist	-5.86	-6.12	-13.94	3.99	42%	-0.26	-5.99	17.93	8.97	-4.98
hex	Red	-8.08	10.11			58%	18.19	1.02			
hex	Red	7.97	-10.24	13.93	-4.00		-18.21	-1.14	-17.93	-8.97	4.97
pent	Twist	6.19	6.45				0.26	6.32			
hex	Sym*	-0.23	-0.21				0.02	-0.22			
	Sum			-0.01	-0.01		-0.02	0.21	0.00	0.00	-0.01

SUPPLEMENT 1 TABLE 1B: Carbon models (continued)

Ring	Edge type	Ext rot (E)	Int rot (I)	$\sum_{\text{half}} E$	$\sum_{\text{half}} I$	Dist of E (α)	DAD (D)	Twist (T)	$\sum_{\text{half}} D$	$\sum_{\text{half}} D/2$	$\sum_{\text{half}} T$
531											
pent	Sym	0.00	0.00				0.00	0.00			
pent	BLUE	-15.81	-2.05	-30.96	1.27	51%	13.76	-8.93	32.23	16.12	-14.85
hex	Red	-15.15	3.32			49%	18.47	-5.92			
hex	Red	15.15	-3.32	30.96	-1.27		-18.47	5.92	-32.23	-16.12	14.85
pent	BLUE	15.81	2.05				-13.76	8.93			
	Sum			0.00	0.00		0.00	0.00	0.00	0.00	0.00
532											
hex	Twist	-6.51	-6.35	-11.38	3.29	57%	0.16	-6.43	14.67	7.34	-4.05
pent	BLUE	-4.87	9.64			43%	14.51	2.39			
pent	BLUE	5.15	-9.24	11.35	-3.29		-14.39	-2.05	-14.64	-7.32	4.03
hex	Twist	5.76	5.31				-0.45	5.54			
pent	Sym*	0.44	0.64				0.20	0.54			
	Sum			-0.03	0.00		-0.17	-0.56	0.03	0.02	-0.01
541											
pent	Twist	-5.55	-5.82	-16.42	-2.22	34%	-0.27	-5.69	14.20	7.10	-9.32
pent	BLUE	-10.87	3.60			66%	14.47	-3.64			
hex	Sym	0.00	0.00				0.00	0.00			
pent	BLUE	10.87	-3.60	16.42	2.22		-14.47	3.64	-14.20	-7.10	9.32
pent	Twist	5.55	5.82				0.27	5.69			
	Sum			0.00	0.00		0.00	0.00	0.27	0.00	0.00

Supplement 1 Table 1B. Angles of interest (in degrees) associated with all of the edges of all the hex-Rings and pent-Rings composed of carbon atoms.

Edge lengths were constrained to 1.43 Å. Internal angles were constrained to 108° in pentagonal faces and 120° in hexagonal faces. All bonds were single bonds, but electrostatic interactions were turned off. The equilibrium geometry of each Ring structure was determined by molecular mechanics calculations (MMFF94) (20-24) in Spartan '04. External rotation (E) and internal rotation (I) were measured. DAD (D) and twist (T) were calculated from E and I according to Eqs. 1 and 2.