



Supporting Information

© Wiley-VCH 2005

69451 Weinheim, Germany

## Harder than Diamond; Determining the Cross Section Area and Young's Modulus of Molecular Rods

Lior Itzhaki, Eli Altus, Harold Basch and Shmaryahu Hoz\*

Computational results.

**C<sub>n</sub>H<sub>2</sub>**

n	The free		A point before the buckling		Buckling point		A point after the buckling	
	length (Å)	Energy (a.u.)	distance (Å)	Energy (a.u.)	distance (Å)	Energy (a.u.)	distance (Å)	Energy (a.u.)
4	3.8035	-153.4513991	3.723	-153.4480383	3.72	-153.4477735	3.62	-153.4393278
6	6.3878	-229.5936195	6.35	-229.5932078	6.34	-229.5929585	6.24	-229.5899415
8	8.9686	-305.7371463	8.95	-305.7370776	8.94	-305.7369823	8.84	-305.7356154
10	11.5473	-381.8812163	11.53	-381.8811717	11.52	-381.8811031	11.42	-381.8802859
12	14.1243	-458.025527	14.109	-458.025496	14.095	-458.0254249	13.995	-458.0248754
14	16.7014	-534.1699481	16.69	-534.169934	16.67	-534.1698609	16.57	-534.1694661
16	19.2778	-610.3144254	19.26	-610.3143961	19.24	-610.314337	19.14	-610.3140387
18	21.8544	-686.4589333	21.83	-686.4588943	21.81	-686.458848	21.71	-686.4586155
20	24.4301	-762.6034593	24.42	-762.6034519	24.4	-762.6034153	24.3	-762.6032306

**[n]staffanes**

n	The free		A point before the buckling		Buckling point		A point after the buckling	
	length (Å)	Energy (a.u.)	distance (Å)	Energy (a.u.)	distance (Å)	Energy (a.u.)	distance (Å)	Energy (a.u.)
3	8.7098	-583.2269063	8.56	-583.2241532	8.55	-583.2237633	8.45	-583.2195795
4	12.1121	-777.2391804	11.98	-777.2376019	11.97	-777.2373533	11.87	-777.2353652

