



Supplementary Information

From Cyclo[18]carbon to the Novel Nanostructures. Theoretical Predictions.

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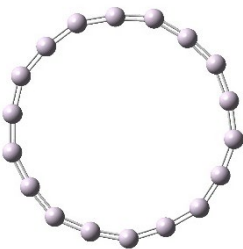
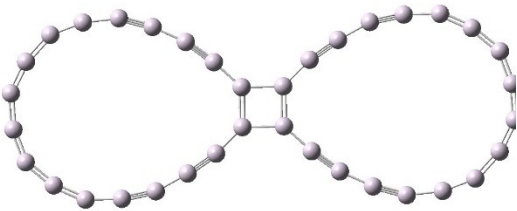
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Table S1. The energy and the lowest vibrational frequency values obtained at the DFT/B3LYP/6-31g-dp level for the isomers of C₁₈, C₃₆ and C₇₂.

Structure	E[au]	ν_{\min} [cm ⁻¹]	Symmetry
^{S0} C ₁₈	-685.358037	60.8	D _{18h}
^{S0} C ₁₈ (TS)	-685.226415	-454.5	C _{2v}
^{S0} C ₃₆	-1370.7748909	19.7	C _{2h}
^{S0} C ₇₂ -ribbon	-2741.592654	12.8	C ₁
^{S0} C ₇₂ -sheet	-2741.656951	14.2	C _{2h}
^{S1} C ₁₈	-685.2475122	54.16	C _{2v}
^{S1} C ₃₆ -ribbon	-1370.6688861	22.4	C _{2v}
^{S1} C ₃₆ -sheet	-1370.6890768	25.4	D _{2h}
^{S1} C ₇₂ -sheet-1	-2741.602896	14.9	D _{2h}
^{S1} C ₇₂ -sheet-2	-2741.545390	15.3	C _{2v}
^{S1} C ₇₂ -tube-1	-2741.611567	39.6	C _{2v}
^{S1} C ₇₂ -tube-2	-2741.636157	36.4	C _{2h}
^{S2} C ₁₈	-685.128517	37.7	C _{2v}

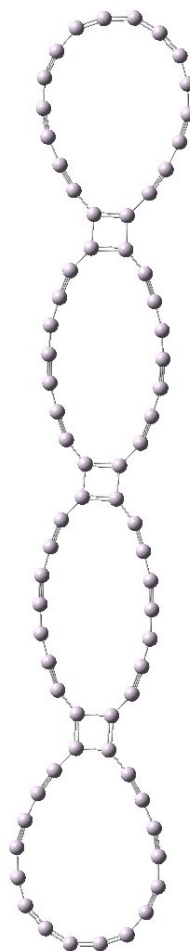
$S^2C_{18}(TS1)$	-685.198184	-190.3	C_2
S^2C_{18-int}	-685.200911	46.4	C_2
$S^2C_{18}(TS2)$	-685.126754	-519.1	C_{2v}
$S^2C_{36-ribbon-1}$	-1370.546734	17.25	C_{2v}
$S^2C_{36-ribbon-1}(TS)$	-1370.518246	-317.9	C_{2v}
$S^2C_{36-ribbon-2}$	-1370.529725	13.0	C_{2v}
$S^2C_{72-ribbon}$	-2741.207540	13.6	D_{2h}
$S^2C_{36-sheet}$	-1370.596843	47.4	C_1
$S^2C_{72-sheet-1}$	-2741.190539	25.7	D_{2h}
$S^2C_{72-sheet-2}$	-2741.420583	10.6	C_1
$S^2C_{72-tube}$	-2741.375611	38.4	C_{2v}

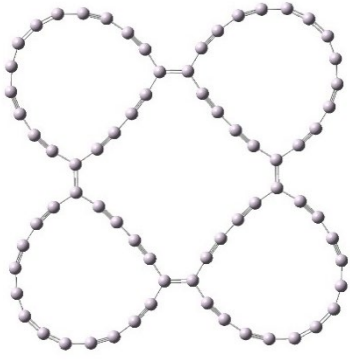
Table S2. The Cartesian coordinates (X,Y,Z) for the generated structures (C18, C36 and C72).

1.	S^0C_{18}				
	1 c	0.224210	-3.728802	0.000000	
	2 c	-1.040533	-3.497843	0.000000	
	3 c	1.451361	-3.348215	0.000000	
	4 c	-2.225058	-3.000328	0.000000	
	5 c	2.568959	-2.712636	0.000000	
	6 c	-3.045804	-2.010777	0.000000	
	7 c	3.263843	-1.631967	0.000000	
	8 c	-3.633496	-0.868241	0.000000	
	9 c	3.711738	-0.426827	0.000000	
	10 c	-3.625910	0.417344	0.000000	
	11 c	3.549136	0.847715	0.000000	
	12 c	-3.341465	1.670300	0.000000	
	13 c	3.117713	2.058810	0.000000	
	14 c	-2.509121	2.650066	0.000000	
	15 c	2.174016	2.930783	0.000000	
	16 c	-1.485931	3.427210	0.000000	
	17 c	1.064866	3.580815	0.000000	
	18 c	-0.218524	3.642595	0.000000	
2.	S^0C_{36}				
	1 c	-5.091829	-3.326623	0.000000	
	2 c	-6.405348	-3.354966	0.000000	
	3 c	-3.865552	-3.053551	0.000000	
	4 c	-7.554743	-2.839837	0.000000	
	5 c	-2.716232	-2.411617	0.000000	
	6 c	-8.569416	-2.006459	0.000000	
	7 c	-1.690713	-1.695883	0.000000	
	8 c	-9.011327	-0.824660	0.000000	

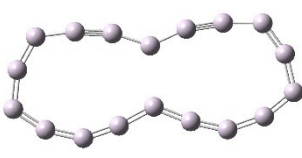
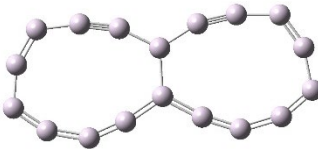
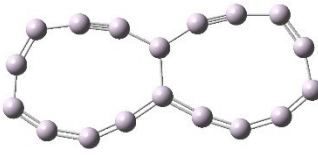
	9 c	-0.737340	-0.739401	0.000000	
	10 c	-9.107449	0.483486	0.000000	
	11 c	-0.766816	0.704686	0.000000	
	12 c	-8.557438	1.619659	0.000000	
	13 c	-1.767978	1.608555	0.000000	
	14 c	-7.679879	2.592895	0.000000	
	15 c	-2.785022	2.337439	0.000000	
	16 c	-6.501596	3.041925	0.000000	
	17 c	-3.982249	2.877798	0.000000	
	18 c	-5.200108	3.193023	0.000000	
	19 c	5.200108	-3.193023	0.000000	
	20 c	3.982249	-2.877798	0.000000	
	21 c	6.501596	-3.041925	0.000000	
	22 c	2.785022	-2.337439	0.000000	
	23 c	7.679879	-2.592895	0.000000	
	24 c	1.767978	-1.608555	0.000000	
	25 c	8.557438	-1.619659	0.000000	
	26 c	0.766816	-0.704686	0.000000	
	27 c	9.107449	-0.483486	0.000000	
	28 c	0.737340	0.739401	0.000000	
	29 c	9.011327	0.824660	0.000000	
	30 c	1.690713	1.695883	0.000000	
	31 c	8.569416	2.006459	0.000000	
	32 c	2.716232	2.411617	0.000000	
	33 c	7.554743	2.839837	0.000000	
	34 c	3.865552	3.053551	0.000000	
	35 c	6.405348	3.354966	0.000000	
	36 c	5.091829	3.326623	0.000000	
3.	⁵⁰ C72-ribbon				

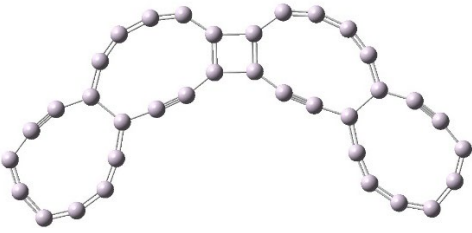
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3 c	-14.703013	-3.570354	0.368167
4 c	-18.404526	-3.478343	0.113315
5 c	-13.535052	-2.949641	0.384146
6 c	-19.469424	-2.708414	-0.007941
7 c	-12.493314	-2.266152	0.362120
8 c	-19.971963	-1.561636	-0.117811
9 c	-11.537506	-1.304951	0.245334
10 c	-20.104782	-0.253039	-
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11 c	-11.607322	0.133057	0.164650
12 c	-19.558346	0.879318	-
0.242591			
13 c	-12.656030	0.997746	0.157569
14 c	-18.655819	1.838132	-
0.243861			
15 c	-13.724526	1.636054	0.095952
16 c	-17.472404	2.256271	-
0.190939			
17 c	-14.949454	2.118525	-
0.005778			
18 c	-16.166061	2.397996	-
0.108813			
19 c	-5.264403	-2.710935	0.512658
20 c	-6.547426	-2.721727	0.394982
21 c	-4.000560	-2.580138	0.603802
22 c	-7.795264	-2.445024	0.266590
23 c	-2.766844	-2.171438	0.622831
24 c	-9.018703	-2.093040	0.159072
25 c	-1.596723	-1.694670	0.582483
26 c	-10.061557	-1.278790	
0.081462			
27 c	-0.633092	-0.773564	0.414443
28 c	-10.135328	0.236035	0.000021
29 c	-0.711637	0.707725	0.386566
30 c	-9.182291	1.156967	-0.005600
31 c	-1.769677	1.529646	0.496134
32 c	-8.001047	1.639127	0.072710
33 c	-2.979130	1.895717	0.482499
34 c	-6.790354	2.054866	0.177531
35 c	-4.245221	2.184366	0.415141
36 c	-5.513871	2.181100	0.302106
37 c	5.546579	-2.236290	0.050679
38 c	4.275169	-2.221977	-0.087250
39 c	6.818843	-2.127520	0.196996
40 c	3.018416	-1.917748	-0.167342
41 c	8.035424	-1.715660	0.309816
42 c	1.808688	-1.536963	-0.185761
43 c	9.209228	-1.224210	0.376262
44 c	0.759403	-0.713910	-0.082912



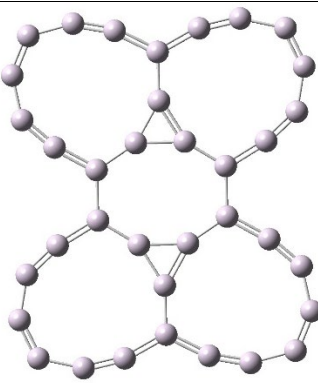
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	46 c	0.683218	0.777582	-0.097436	
	47 c	10.089221	1.200799	0.430860	
	48 c	1.649446	1.699353	-0.187595	
	49 c	9.042028	2.017188	0.492482	
	50 c	2.820806	2.182865	-0.133051	
	51 c	7.828970	2.400673	0.432831	
	52 c	4.044987	2.590953	-0.016654	
	53 c	6.581261	2.703689	0.315808	
	54 c	5.307463	2.708376	0.147732	
	55 c	16.150210	-2.348167	-	
	0.760010				
	56 c	14.931971	-2.090580	-	
	0.622251				
	57 c	17.452043	-2.188273	-	
	0.878776				
	58 c	13.704671	-1.632558	-	
	0.456982				
	59 c	18.628199	-1.756440	-	
	0.967451				
	60 c	12.634129	-1.023837	-	
	0.262685				
	61 c	19.523664	-0.790510	-	
	0.989416				
	62 c	11.601319	-0.179364	-	
	0.000236				
	63 c	20.064420	0.344935	-0.959678	
	64 c	11.528661	1.260492	0.066209	
	65 c	19.924506	1.652880	-0.860096	
	66 c	12.460704	2.238523	-0.094875	
	67 c	19.411390	2.794826	-0.743680	
	68 c	13.484733	2.941614	-0.189704	
	69 c	18.337399	3.549267	-0.600545	
	70 c	14.639983	3.581278	-0.271993	
	71 c	17.163449	3.970930	-0.468742	
	72 c	15.850709	3.884455	-0.358501	
4.	⁵⁰ C ₇₂ -sheet				
	1 c	-5.232917	0.612095	0.000000	
	2 c	-6.435784	1.308533	0.000000	
	3 c	-4.097201	1.400438	0.000000	
	4 c	-7.362765	2.130840	0.000000	
	5 c	-3.196202	2.254206	0.000000	
	6 c	-8.109262	3.228025	0.000000	
	7 c	-2.309285	3.244402	0.000000	
	8 c	-8.577069	4.385188	0.000000	
	9 c	-1.565460	4.238015	0.000000	
	10 c	-8.554127	5.708210	0.000000	
	11 c	-0.855757	5.423735	0.000000	
	12 c	-8.186921	6.904217	0.000000	
	13 c	-1.607299	6.594062	0.000000	
	14 c	-7.253435	7.842923	0.000000	

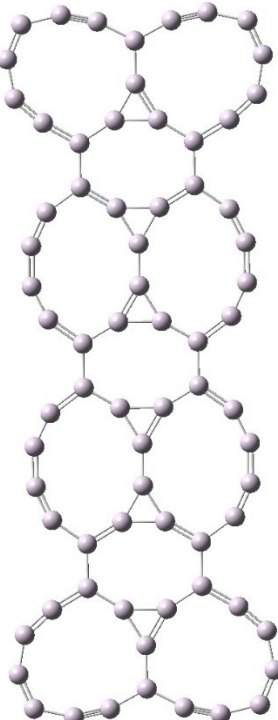
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18	c	-4.824294	8.461113	0.000000
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20	c	4.016606	1.573073	0.000000
21	c	6.357020	1.609831	0.000000
22	c	3.081195	2.388673	0.000000
23	c	7.242546	2.477044	0.000000
24	c	2.151914	3.338240	0.000000
25	c	7.941742	3.604961	0.000000
26	c	1.363655	4.296633	0.000000
27	c	8.356831	4.782291	0.000000
28	c	0.607004	5.453137	0.000000
29	c	8.267669	6.101941	0.000000
30	c	1.306772	6.654832	0.000000
31	c	7.857589	7.283649	0.000000
32	c	2.155189	7.556685	0.000000
33	c	6.884119	8.180245	0.000000
34	c	3.224094	8.349408	0.000000
35	c	5.751565	8.709899	0.000000
36	c	4.427404	8.676318	0.000000
37	c	-4.427404	-8.676318	0.000000
38	c	-5.751565	-8.709899	0.000000
39	c	-3.224094	-8.349408	0.000000
40	c	-6.884119	-8.180245	0.000000
41	c	-2.155189	-7.556685	0.000000
42	c	-7.857589	-7.283649	0.000000
43	c	-1.306772	-6.654832	0.000000
44	c	-8.267669	-6.101941	0.000000
45	c	-0.607004	-5.453137	0.000000
46	c	-8.356831	-4.782291	0.000000
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49	c	-2.151914	-3.338240	0.000000
50	c	-7.242546	-2.477044	0.000000
51	c	-3.081195	-2.388673	0.000000
52	c	-6.357020	-1.609831	0.000000
53	c	-4.016606	-1.573073	0.000000
54	c	-5.193423	-0.848751	0.000000
55	c	4.824294	-8.461113	0.000000
56	c	3.606073	-8.193381	0.000000
57	c	6.149012	-8.429887	0.000000
58	c	2.501606	-7.450813	0.000000
59	c	7.253435	-7.842923	0.000000
60	c	1.607299	-6.594062	0.000000
61	c	8.186921	-6.904217	0.000000
62	c	0.855757	-5.423735	0.000000
63	c	8.554127	-5.708210	0.000000
64	c	1.565460	-4.238015	0.000000
65	c	8.577069	-4.385188	0.000000

	66 c	2.309285	-3.244402	0.000000	
	67 c	8.109262	-3.228025	0.000000	
	68 c	3.196202	-2.254206	0.000000	
	69 c	7.362765	-2.130840	0.000000	
	70 c	4.097201	-1.400438	0.000000	
	71 c	6.435784	-1.308533	0.000000	
	72 c	5.232917	-0.612095	0.000000	
5.	⁵⁰ C ₁₈ (TS)				
	1 c	0.056786	-0.945232	0.000044	
	2 c	-1.114265	-1.581247	0.000093	
	3 c	1.295098	-1.436595	-0.000067	
	4 c	-2.308012	-1.997826	0.000139	
	5 c	2.530368	-1.707727	-0.000158	
	6 c	-3.582086	-1.712738	0.000140	
	7 c	3.760698	-1.272071	-0.000166	
	8 c	-4.661339	-1.022423	0.000096	
	9 c	4.750626	-0.458043	-0.000111	
	10 c	-4.526103	0.292977	-	
	0.000056				
	11 c	4.458053	0.831132	0.000069	
	12 c	-3.907436	1.403868	-	
	0.000178				
	13 c	3.711576	1.860964	0.000211	
	14 c	-2.590720	1.575907	-	
	0.000147				
	15 c	2.384137	1.874220	0.000160	
	16 c	-1.335783	1.517916	-	
	0.000093				
	17 c	1.144665	1.667348	0.000073	
	18 c	-0.066263	1.109571	-	
	0.000050				
6.	⁵¹ C ₁₈				
	1 c	0.040397	-0.673627	0.000000	
	2 c	-1.106155	-1.456587	0.000000	
	3 c	1.272396	-1.313737	0.000000	
	4 c	-2.240352	-1.964862	0.000000	
	5 c	2.459340	-1.682465	0.000000	
	6 c	-3.552517	-1.737710	0.000000	
	7 c	3.734829	-1.299822	0.000000	
	8 c	-4.600823	-1.036310	0.000000	
	9 c	4.691938	-0.478274	0.000000	
	10 c	-4.501763	0.304095	0.000000	
	11 c	4.432740	0.840556	0.000000	
	12 c	-3.883510	1.396973	0.000000	
	13 c	3.688609	1.851936	0.000000	
	14 c	-2.537750	1.564534	0.000000	
	15 c	2.332421	1.856763	0.000000	
	16 c	-1.308217	1.427889	0.000000	
	17 c	1.128019	1.574144	0.000000	
	18 c	-0.049602	0.826504	0.000000	

7.	⁵¹ C ₃₆ -ribbon				
	1 c	-4.272835	-0.461607	0.000000	
	2 c	-4.495305	-1.836873	0.000000	
	3 c	-2.974580	0.019335	0.000000	
	4 c	-4.916130	-3.004344	0.000000	
	5 c	-1.850848	0.542956	0.000000	
	6 c	-5.988997	-3.797815	0.000000	
	7 c	-0.791062	1.401203	0.000000	
	8 c	-7.217133	-4.078264	0.000000	
	9 c	-0.820282	2.829164	0.000000	
	10 c	-8.123263	-3.082722	0.000000	
	11 c	-1.966898	3.572448	0.000000	
	12 c	-8.504503	-1.887172	0.000000	
	13 c	-3.209939	3.444228	0.000000	
	14 c	-7.698589	-0.793775	0.000000	
	15 c	-4.389223	2.833014	0.000000	
	16 c	-6.763303	0.015061	0.000000	
	17 c	-5.107014	1.819253	0.000000	
	18 c	-5.446603	0.479510	0.000000	
	19 c	4.288915	-0.261581	0.000000	
	20 c	2.969716	0.158439	0.000000	
	21 c	4.575753	-1.624913	0.000000	
	22 c	1.822711	0.628909	0.000000	
	23 c	5.053490	-2.770183	0.000000	
	24 c	0.723949	1.436681	0.000000	
	25 c	6.162403	-3.512607	0.000000	
	26 c	0.685873	2.864492	0.000000	
	27 c	7.402601	-3.732528	0.000000	
	28 c	1.796201	3.660956	0.000000	
	29 c	8.262005	-2.696405	0.000000	
	30 c	3.043883	3.590701	0.000000	
	31 c	8.584419	-1.483808	0.000000	
	32 c	4.250455	3.035324	0.000000	
	33 c	7.728005	-0.429603	0.000000	
	34 c	5.014763	2.056143	0.000000	
	35 c	6.754287	0.332471	0.000000	
	36 c	5.417079	0.733911	0.000000	
8.	⁵¹ C ₃₆ -sheet				

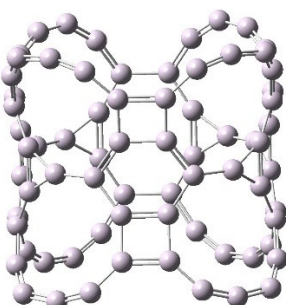
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23 c	1.862606	0.797014	0.000000
24 c	-3.135457	1.340592	0.000000
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27 c	3.941910	2.388370	0.000000
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30 c	-3.897808	4.601918	0.000000
31 c	3.610271	4.833828	0.000000
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33 c	2.287376	5.115852	0.000000
34 c	-1.380602	4.752933	0.000000
35 c	1.086526	4.828921	0.000000
36 c	-0.126870	4.135490	0.000000



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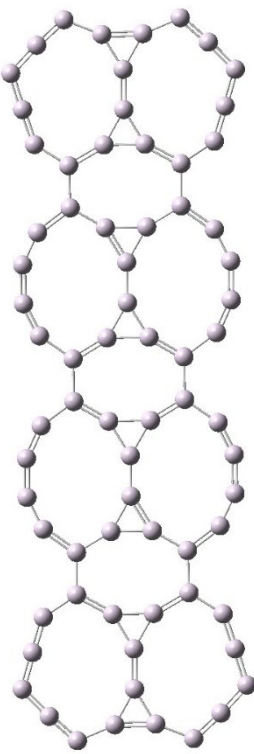
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	55 c	-0.171638	9.370148	
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	67 c	3.559321	11.473713	
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	70 c	-1.437537	11.446032	
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10	SIC72-tube-1			

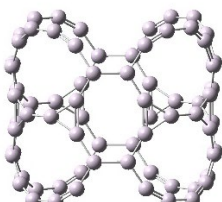
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8 c	-3.757360	-2.858803	
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3.476140			
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11 c	3.791183	-3.726003	
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12 c	-2.898166	-4.086322	
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13 c	3.067451	-3.955978	
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14 c	-1.791560	-4.026480	
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15 c	1.961680	-3.945344	
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16 c	-0.615503	-3.583134	
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17 c	0.764622	-3.555062	
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18 c	0.056682	-2.733697	
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19 c	0.076726	-3.403234	-
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20 c	-0.628220	-3.866114	-
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21 c	0.798542	-3.835002	-
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22 c	-1.801203	-4.036239	-
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23 c	1.975606	-3.954411	-
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24 c	-2.994926	-3.873435	-
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25 c	3.163800	-3.741957	-
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31 c	3.068733	-1.427321	-
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33 c	1.919335	-0.716474	-
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34 c	-0.682612	-1.489769	-
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37 c	-0.048463	2.494792	-
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38 c	-0.744446	1.415433	-
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39 c	0.694920	1.446498	-
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45 c	3.635723	2.414682	-
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48 c	-3.157319	3.725734	-
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	53 c	0.634069	3.850347	-
	1.369051			
	54 c	-0.068365	3.376447	-
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	58 c	-1.963539	3.954450	
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	61 c	2.893101	4.102026	
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	69 c	2.534924	0.812996	
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11	SIC72-sheet-2			

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	14 c	7.416517	-1.935697	-
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	16 c	8.109971	-0.704109	
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	0.030574			
	22 c	5.954220	-1.911375	-
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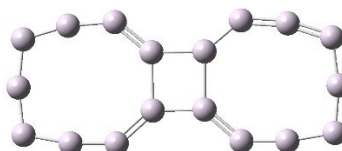
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29 c	2.671497	3.577107	-
0.042533			
30 c	1.555011	-3.049630	-
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31 c	1.555011	3.049630	-
0.048754			
32 c	0.734894	-1.909181	-
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33 c	0.734894	1.909181	-
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34 c	1.437613	-0.719837	-
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0.055119			
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0.053861			
42 c	-1.555011	-3.049630	-
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43 c	-1.555011	3.049630	-
0.048754			
44 c	-2.671497	-3.577107	-
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45 c	-2.671497	3.577107	-
0.042533			
46 c	-4.015993	-3.585414	-
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48 c	-5.125183	-3.043555	-
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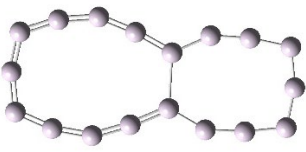
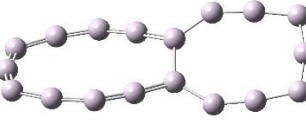
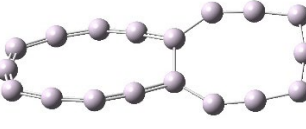
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12	⁵¹ C _{72-tube-2}	
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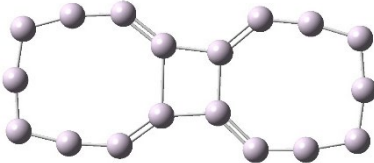
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7 c	3.050475	-1.409729	-
3.945226			
8 c	-3.635794	-2.367150	-
3.388783			
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2.412263			
11 c	3.647619	-3.252160	-
2.410904			
12 c	-3.029296	-3.892967	-
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13 c	3.082759	-3.853029	-
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14 c	-1.869203	-4.182526	-
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15 c	1.926060	-4.156986	-
0.751221			
16 c	-0.685421	-4.018956	-
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17 c	0.740534	-4.009337	-
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18 c	0.024190	-3.481282	-
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21 c	0.740389	-4.046303	
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1.449053			
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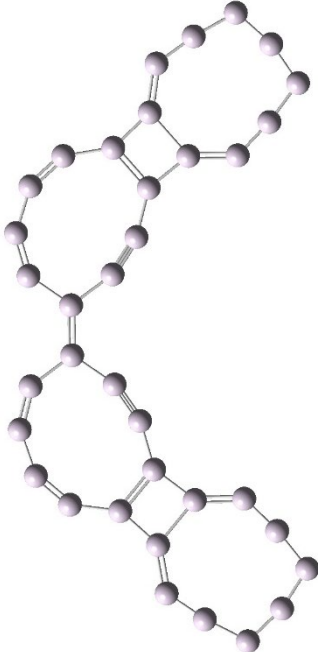
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31 c	3.048227	-1.493725
3.937928		
32 c	-1.893481	-0.782594
4.271804		
33 c	1.901210	-0.757422
4.273559		
34 c	-0.703563	-1.502031
4.127163		
35 c	0.721052	-1.492673
4.128014		
36 c	0.016274	-2.571029
3.562820		
37 c	-0.017687	2.491164
3.582848		
38 c	-0.723059	1.405975
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39 c	0.701889	1.415347
4.134293		
40 c	-1.902987	0.670342
4.274659		
41 c	1.891310	0.695463
4.275618		
42 c	-3.050475	1.409729
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43 c	3.029339	1.449941
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44 c	-3.669602	2.319416
3.388465		
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3.388783		
46 c	-3.647619	3.252160
2.410904		
47 c	3.602908	3.300720
2.412263		
48 c	-3.082759	3.853029
1.495638		
49 c	3.029296	3.892967
1.496820		
50 c	-1.926060	4.156986
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51 c	1.869203	4.182526
0.752110		
52 c	-0.740534	4.009337
1.475105		
53 c	0.685421	4.018956
1.475444		

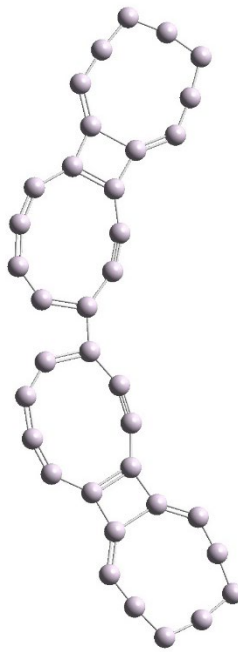
	54 c	-0.024190	3.481282	
	2.564793			
	55 c	-0.023322	3.543491	-
	2.527204			
	56 c	-0.740389	4.046303	-
	1.425917			
	57 c	0.686110	4.056049	-
	1.425589			
	58 c	-1.926169	4.175531	-
	0.698952			
	59 c	1.869719	4.201475	-
	0.698076			
	60 c	-3.084281	3.890811	-
	1.449053			
	61 c	3.031742	3.932743	-
	1.447911			
	62 c	-3.648107	3.306012	-
	2.375000			
	63 c	3.604323	3.356112	-
	2.373618			
	64 c	-3.673773	2.392170	-
	3.370064			
	65 c	3.642379	2.442525	-
	3.368557			
	66 c	-3.048227	1.493725	-
	3.937928			
	67 c	3.030406	1.534060	-
	3.935345			
	68 c	-1.901210	0.757422	-
	4.273559			
	69 c	1.893481	0.782594	-
	4.271804			
	70 c	-0.721052	1.492673	-
	4.128014			
	71 c	0.703563	1.502031	-
	4.127163			
	72 c	-0.016274	2.571029	-
	3.562820			
13	S ² C ₁₈			
	1 c	-0.721595	0.000000	-0.729585
	2 c	0.721595	0.000000	-0.729585
	3 c	-1.731979	0.000000	-1.605633
	4 c	1.731979	0.000000	-1.605633
	5 c	-3.014192	0.000000	-1.602289
	6 c	3.014192	0.000000	-1.602289
	7 c	-4.325377	0.000000	-1.379802
	8 c	4.325377	0.000000	-1.379802
	9 c	-4.443712	0.000000	-0.082012
	10 c	4.443712	0.000000	-0.082012
	11 c	-4.291848	0.000000	1.229492
	12 c	4.291848	0.000000	1.229492



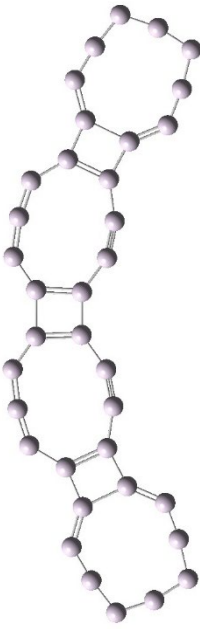
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	14 c	3.050804	0.000000	1.607466	
	15 c	-1.752706	0.000000	1.699829	
	16 c	1.752706	0.000000	1.699829	
	17 c	-0.735091	0.000000	0.862533	
	18 c	0.735091	0.000000	0.862533	
14	s^2C_{18} (TS1)				
	1 c	0.481533	-0.954170	0.000000	
	2 c	-0.781672	-1.402172	0.000000	
	3 c	1.607228	-1.703532	0.000000	
	4 c	-2.020011	-1.679490	0.000000	
	5 c	2.864244	-1.837111	0.000000	
	6 c	-3.279589	-1.376456	0.000000	
	7 c	4.199496	-1.783781	0.000000	
	8 c	-4.428811	-0.782373	0.000000	
	9 c	4.542358	-0.522936	0.000000	
	10 c	-4.481608	0.516007	0.000000	
	11 c	4.495241	0.782844	0.000000	
	12 c	-4.135133	1.768432	0.000000	
	13 c	3.207029	1.138273	0.000000	
	14 c	-2.880932	2.085693	0.000000	
	15 c	1.952534	1.293512	0.000000	
	16 c	-1.585450	2.094338	0.000000	
	17 c	0.685967	0.819823	0.000000	
	18 c	-0.442423	1.543100	0.000000	
15	$s^2C_{18}^{prim}$				
	1 c	0.482352	-0.837350	-	
		0.137773			
	2 c	-0.748480	-1.336390		
		0.129027			
	3 c	1.550066	-1.658564	-	
		0.471933			
	4 c	-1.955870	-1.653614		
		0.363952			
	5 c	2.803811	-1.772843	-	
		0.452398			
	6 c	-3.215505	-1.352473		
		0.396551			
	7 c	4.147212	-1.729068	-	
		0.364315			
	8 c	-4.355827	-0.740563		
		0.343083			
	9 c	4.459375	-0.511228	-	
		0.003572			
	10 c	-4.426401	0.510065	-	
		0.000348			
	11 c	4.431504	0.745291		
		0.358769			
	12 c	-4.073184	1.711739	-	
		0.343346			

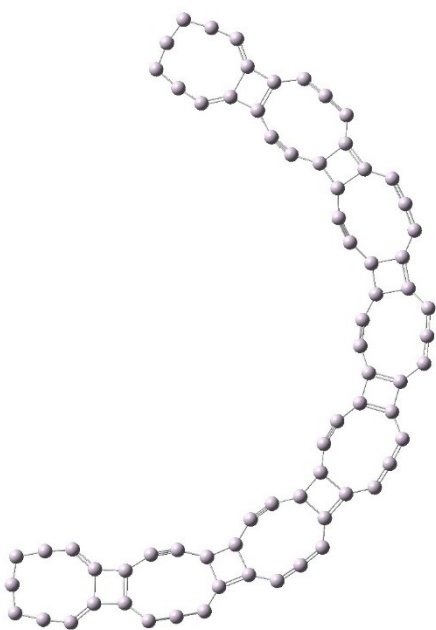
	13 c 3.132813 1.090723 0.450370 14 c -2.823171 2.047758 - 0.395511 15 c 1.885547 1.261289 0.473454 16 c -1.528278 2.053518 - 0.361436 17 c 0.659359 0.702783 0.141149 18 c -0.425324 1.468929 - 0.125722	
16	^{S2} C ₁₈ (TS2)	
	1 c 0.642158 -0.815216 0.000000 2 c -0.795534 -0.763911 0.000000 3 c 1.523138 -1.831355 0.000000 4 c -1.923110 -1.433900 0.000000 5 c 2.802117 -1.931722 0.000000 6 c -3.204408 -1.265062 0.000000 7 c 4.123088 -1.819948 0.000000 8 c -4.452341 -0.850067 0.000000 9 c 4.407989 -0.545664 0.000000 10 c -4.424936 0.456913 0.000000 11 c 4.419796 0.770538 0.000000 12 c -4.114897 1.732987 0.000000 13 c 3.200038 1.244639 0.000000 14 c -2.837752 1.961408 0.000000 15 c 1.927049 1.472653 0.000000 16 c -1.536906 1.899682 0.000000 17 c 0.832675 0.711244 0.000000 18 c -0.588164 1.006782 0.000000	
17	^{S2} C _{36-ribbon-1}	

	1 c	-5.982701	0.057665	
	0.000000			
	2 c	-5.017452	1.076658	
	0.000000			
	3 c	-7.331697	-0.143554	
	0.000000			
	4 c	-4.806914	2.461461	
	0.000000			
	5 c	-8.072773	-1.179468	
	0.000000			
	6 c	-3.983533	3.381415	
	0.000000			
	7 c	-8.709872	-2.352391	
	0.000000			
	8 c	-2.690708	3.792558	
	0.000000			
	9 c	-7.830993	-3.320672	
	0.000000			
	10 c	-1.501810	3.461354	
	0.000000			
	11 c	-6.745092	-4.046595	
	0.000000			
	12 c	-0.677299	2.293842	
	0.000000			
	13 c	-5.678111	-3.242283	
	0.000000			
	14 c	-1.514203	1.140709	
	0.000000			
	15 c	-4.765819	-2.355075	
	0.000000			
	16 c	-2.539652	0.466719	
	0.000000			
	17 c	-4.765638	-0.990626	
	0.000000			
	18 c	-3.894518	0.111372	
	0.000000			
	19 c	5.032210	1.005467	
	0.000000			
	20 c	5.982906	-0.027108	
	0.000000			
	21 c	4.841482	2.393167	
	0.000000			
	22 c	7.328915	-0.247427	
	0.000000			
	23 c	4.030907	3.324423	
	0.000000			
	24 c	8.055222	-1.293741	
	0.000000			
	25 c	2.744180	3.754261	
	0.000000			

	26 c 8.675658 -2.475556 0.000000 27 c 1.550843 3.439486 0.000000 28 c 7.783168 -3.431306 0.000000 29 c 0.709678 2.283944 0.000000 30 c 6.687099 -4.141782 0.000000 31 c 1.530098 1.119036 0.000000 32 c 5.631608 -3.322429 0.000000 33 c 2.545997 0.430718 0.000000 34 c 4.731988 -2.422377 0.000000 35 c 3.895707 0.056191 0.000000 36 c 4.751119 -1.058054 0.000000	
18	^{S2} C ₃₆ -ribbon-1 (TS)	
	1 c 6.361480 0.000000 0.389191 2 c 5.116854 0.000000 1.043993 3 c 7.701391 0.000000 0.636969 4 c 4.493342 0.000000 2.295773 5 c 8.740215 0.000000 - 0.102457 6 c 3.369690 0.000000 2.831375 7 c 9.724073 0.000000 - 1.001751 8 c 2.038929 0.000000 2.961851 9 c 9.208609 0.000000 - 2.205462 10 c 0.975408 0.000000 2.275578 11 c 8.419501 0.000000 - 3.244695 12 c 0.698129 0.000000 0.846165 13 c 7.148436 0.000000 - 2.829206 14 c 1.786845 0.000000 - 0.034707	

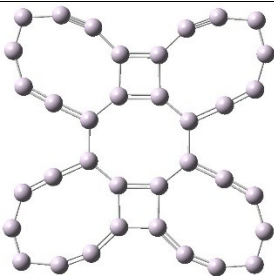
	15 c	5.996880	0.000000	-	
	2.288388				
	16 c	2.979267	0.000000	-	
	0.336089				
	17 c	5.554510	0.000000	-	
	0.997897				
	18 c	4.371291	0.000000	-	
	0.240243				
	19 c	-5.116854	0.000000		
	1.043993				
	20 c	-6.361480	0.000000		
	0.389191				
	21 c	-4.493342	0.000000		
	2.295773				
	22 c	-7.701391	0.000000		
	0.636969				
	23 c	-3.369690	0.000000		
	2.831375				
	24 c	-8.740215	0.000000	-	
	0.102457				
	25 c	-2.038929	0.000000		
	2.961851				
	26 c	-9.724073	0.000000	-	
	1.001751				
	27 c	-0.975408	0.000000		
	2.275578				
	28 c	-9.208609	0.000000	-	
	2.205462				
	29 c	-0.698129	0.000000		
	0.846165				
	30 c	-8.419501	0.000000	-	
	3.244695				
	31 c	-1.786845	0.000000	-	
	0.034707				
	32 c	-7.148436	0.000000	-	
	2.829206				
	33 c	-2.979267	0.000000	-	
	0.336089				
	34 c	-5.996880	0.000000	-	
	2.288388				
	35 c	-4.371291	0.000000	-	
	0.240243				
	36 c	-5.554510	0.000000	-	
	0.997897				
19	S2C ₃₆ -ribbon-2				

	1 c	-6.346158	0.499388	
	0.000000			
	2 c	-5.048172	1.051790	
	0.000000			
	3 c	-7.657577	0.863348	
	0.000000			
	4 c	-4.333071	2.244795	
	0.000000			
	5 c	-8.758334	0.216921	
	0.000000			
	6 c	-3.132125	2.628220	
	0.000000			
	7 c	-9.814167	-0.594094	
	0.000000			
	8 c	-1.825710	2.786874	
	0.000000			
	9 c	-9.403279	-1.838432	
	0.000000			
	10 c	-0.751720	2.031831	
	0.000000			
	11 c	-8.707061	-2.941256	
	0.000000			
	12 c	-0.701584	0.536507	
	0.000000			
	13 c	-7.404823	-2.638580	
	0.000000			
	14 c	-1.829734	-0.268679	
	0.000000			
	15 c	-6.211060	-2.196839	
	0.000000			
	16 c	-3.040677	-0.500398	
	0.000000			
	17 c	-5.662683	-0.948643	
	0.000000			
	18 c	-4.415291	-0.298177	
	0.000000			
	19 c	5.061586	0.984285	
	0.000000			
	20 c	6.352038	0.414572	
	0.000000			
	21 c	4.362909	2.187118	
	0.000000			
	22 c	7.668250	0.760881	
	0.000000			
	23 c	3.166760	2.585345	
	0.000000			
	24 c	8.760352	0.099945	
	0.000000			
	25 c	1.862644	2.763045	
	0.000000			

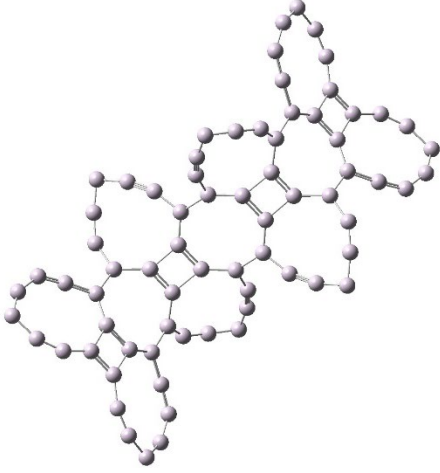
	26 c 9.805366 -0.724940 0.000000 27 c 0.779152 2.021614 0.000000 28 c 9.377946 -1.963757 0.000000 29 c 0.708842 0.527122 0.000000 30 c 8.667191 -3.057222 0.000000 31 c 1.825934 -0.293295 0.000000 32 c 7.369025 -2.737132 0.000000 33 c 3.033685 -0.541136 0.000000 34 c 6.181278 -2.279609 0.000000 35 c 4.410850 -0.357212 0.000000 36 c 5.649417 -1.024200 0.000000	
20	^{S2} C ₇₂ -ribbon	
	1 c 12.076686 0.601763 - 6.276475 2 c 11.900566 0.439032 - 4.881238 3 c 13.050442 0.737776 - 7.220348 4 c 12.587990 0.242934 - 3.691029 5 c 13.057793 0.846400 - 8.491569 6 c 12.243134 0.261947 - 2.462811 7 c 12.902539 0.940524 - 9.811315 8 c 11.812571 0.122062 - 1.230061 9 c 11.621966 0.915933 - 10.096897 10 c 10.588921 0.293576 - 0.695893 11 c 10.321017 0.851732 - 10.067734 12 c 9.282617 0.370977 - 1.416320 13 c 9.923473 0.750624 - 8.790198 14 c 9.150301 0.386448 - 2.790361	

15 c	9.702436	0.639594	-
7.545340			
16 c	9.531499	0.409517	-
3.963935			
17 c	10.494096	0.581828	-
6.430485			
18 c	10.407904	0.460778	-
5.035618			
19 c	6.869074	-0.738760	
3.657112			
20 c	5.656494	-0.879326	
4.464773			
21 c	8.196145	-0.452190	
3.725902			
22 c	5.165870	-0.767992	
5.706404			
23 c	9.125999	-0.206439	
2.878225			
24 c	3.962494	-0.714175	
6.193785			
25 c	9.946703	0.074039	
1.910064			
26 c	2.741643	-0.643891	
6.597443			
27 c	9.843712	0.233683	
0.591266			
28 c	1.555209	-0.613211	
5.926288			
29 c	8.554559	0.270659	-
0.204408			
30 c	1.352306	-0.542053	
4.431300			
31 c	7.340652	-0.089833	
0.318902			
32 c	2.352770	-0.665815	
3.532231			
33 c	6.543943	-0.503713	
1.177362			
34 c	3.509380	-0.869105	
3.094910			
35 c	6.064145	-0.852964	
2.412652			
36 c	4.850700	-1.013140	
3.165289			
37 c	-4.199160	-0.199412	
5.804150			
38 c	-5.590903	-0.228977	
5.342537			
39 c	-3.394112	-0.441904	
6.852476			

40 c	-6.853841	-0.529221	
5.735438			
41 c	-2.122454	-0.590444	
7.019159			
42 c	-7.986630	-0.595827	
5.124943			
43 c	-0.834599	-0.699767	
7.078679			
44 c	-9.053674	-0.703228	
4.397918			
45 c	0.125910	-0.682659	
6.121698			
46 c	-9.313134	-0.597348	
3.088524			
47 c	-0.079029	-0.544820	
4.617529			
48 c	-8.280551	-0.516652	
1.968947			
49 c	-1.265982	-0.264699	
4.045741			
50 c	-6.960477	-0.267964	
2.196320			
51 c	-2.487510	0.009174	
3.960695			
52 c	-5.936201	-0.020884	
2.863158			
53 c	-3.759953	0.144689	
4.392044			
54 c	-5.139616	0.103626	
3.959907			
55 c	-12.786877	0.355816	-
1.473621			
56 c	-13.357566	0.420118	-
2.768419			
57 c	-13.117889	0.337130	-
0.126149			
58 c	-14.563741	0.406050	-
3.404705			
59 c	-12.421509	0.064024	
0.914112			
60 c	-14.941938	0.492645	-
4.619394			
61 c	-11.685673	-0.053526	
1.994489			
62 c	-15.177801	0.604604	-
5.926551			
63 c	-10.366758	-0.367559	
2.086855			
64 c	-14.033308	0.699222	-
6.562083			

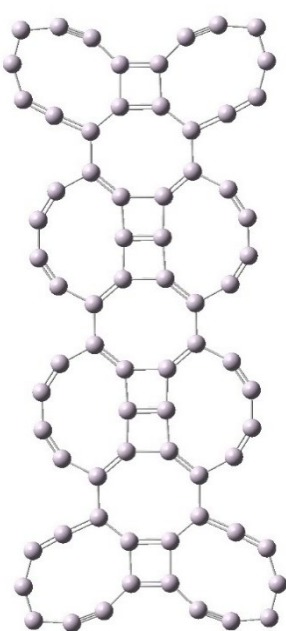
	65 c -9.323066 -0.332816 1.020083 66 c -12.778461 0.787090 - 6.900986 67 c -9.569977 -0.043042 - 0.304626 68 c -12.028908 0.697209 - 5.789986 69 c -10.254116 0.200190 - 1.303590 70 c -11.457292 0.619645 - 4.660519 71 c -11.400538 0.371515 - 2.059381 72 c -11.890415 0.488785 - 3.367267	
21	⁵² C ₃₆ -sheet	
	1 c -0.698665 0.000000 - 3.121878 2 c 0.698665 0.000000 - 3.121878 3 c -1.688698 0.000000 - 4.089939 4 c 1.688698 0.000000 - 4.089939 5 c -2.848464 0.000000 - 4.517581 6 c 2.848464 0.000000 - 4.517581 7 c -4.221104 0.000000 - 4.418998 8 c 4.221104 0.000000 - 4.418998 9 c -4.563099 0.000000 - 3.207836 10 c 4.563099 0.000000 - 3.207836 11 c -4.191843 0.000000 - 1.917505 12 c 4.191843 0.000000 - 1.917505 13 c -3.095871 0.000000 - 1.332320 14 c 3.095871 0.000000 - 1.332320 15 c -1.809077 0.000000 - 0.742060 16 c 1.809077 0.000000 - 0.742060 17 c -0.738111 0.000000 - 1.613297	

	18 c	0.738111	0.000000	-	
	1.613297				
	19 c	-0.737666	0.000000		
	1.613024				
	20 c	0.737666	0.000000		
	1.613024				
	21 c	-1.809138	0.000000		
	0.742496				
	22 c	1.809138	0.000000		
	0.742496				
	23 c	-3.095668	0.000000		
	1.334244				
	24 c	3.095668	0.000000		
	1.334244				
	25 c	-4.191289	0.000000		
	1.919272				
	26 c	4.191289	0.000000		
	1.919272				
	27 c	-4.571977	0.000000		
	3.207647				
	28 c	4.571977	0.000000		
	3.207647				
	29 c	-4.219102	0.000000		
	4.414525				
	30 c	4.219102	0.000000		
	4.414525				
	31 c	-2.848069	0.000000		
	4.521681				
	32 c	2.848069	0.000000		
	4.521681				
	33 c	-1.691040	0.000000		
	4.086763				
	34 c	1.691040	0.000000		
	4.086763				
	35 c	-0.698620	0.000000		
	3.121763				
	36 c	0.698620	0.000000		
	3.121763				
22	S ² C ₇₂ -sheet-1				

1 c	-0.789571	-7.278273	-	
0.700502				
2 c	-0.789571	-7.278273		
0.700502				
3 c	-1.187509	-8.142904	-	
1.697499				
4 c	-1.187509	-8.142904		
1.697499				
5 c	-1.159392	-8.572190	-	
2.860910				
6 c	-1.159392	-8.572190		
2.860910				
7 c	-0.810025	-8.620851	-	
4.182634				
8 c	-0.810025	-8.620851		
4.182634				
9 c	0.007903	-7.694400	-	
4.443219				
10 c	0.007903	-7.694400		
4.443219				
11 c	0.663262	-6.592300	-	
4.066475				
12 c	0.663262	-6.592300		
4.066475				
13 c	0.779106	-5.971576	-	
2.994035				
14 c	0.779106	-5.971576		
2.994035				
15 c	0.763944	-5.350157	-	
1.727669				
16 c	0.763944	-5.350157		
1.727669				
17 c	0.050663	-6.006154	-	
0.715452				
18 c	0.050663	-6.006154		
0.715452				
19 c	1.142070	-3.026655	-	
0.692007				
20 c	1.142070	-3.026655		
0.692007				
21 c	1.460414	-4.071339	-	
1.681525				
22 c	1.460414	-4.071339		
1.681525				
23 c	2.298468	-3.801806	-	
2.735089				
24 c	2.298468	-3.801806		
2.735089				
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3.569282				

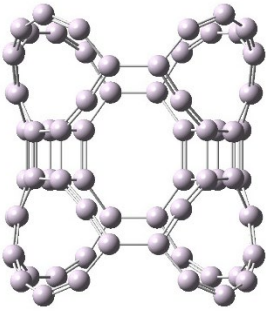
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30 c	1.979866	-1.155932	
3.722752			
31 c	1.125485	-0.722816	-
2.914832			
32 c	1.125485	-0.722816	
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33 c	0.456068	-0.597772	-
1.717344			
34 c	0.456068	-0.597772	
1.717344			
35 c	0.695872	-1.564916	-
0.713977			
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0.713977			
37 c	-0.695872	1.564916	-
0.713977			
38 c	-0.695872	1.564916	
0.713977			
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1.717344			
40 c	-0.456068	0.597772	
1.717344			
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3.722752			
44 c	-1.979866	1.155932	
3.722752			
45 c	-2.868227	1.914241	-
4.427576			
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4.427576			
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	4.182634				
	67 c	1.159392	8.572190	-	
	2.860910				
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	2.860910				
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	1.543712			
	15 c	-3.484324	-1.836943	
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	16 c	-3.484324	1.836943	
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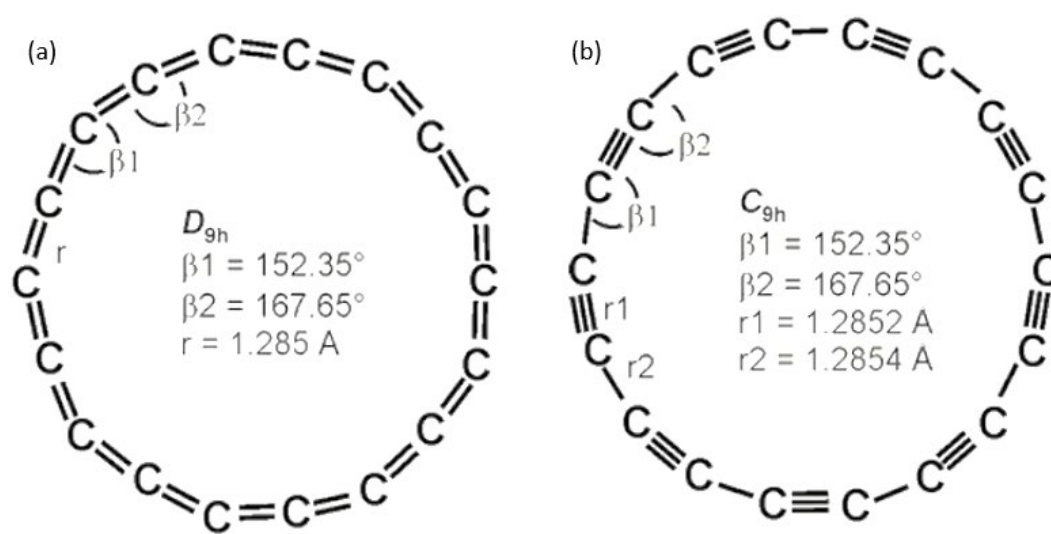


Figure S1. Quantum chemistry calculated^a structures for cyclo[18]carbon; (a) cumulenic; (b) polyynic.

^a Gas-phase electronic spectra of C 18 and C 22 rings

Boguslavskiy, A.E.; Ding, H.; Maier, J.P. Gas-phase electronic spectra of C18 and C22 rings. *J. Chem. Phys.* **2005**, *123*, 034305. <https://doi.org/10.1063/1.1961564>