Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for: Extreme Electron Transport Suppression in Siloxane Ring-based Molecular Devices

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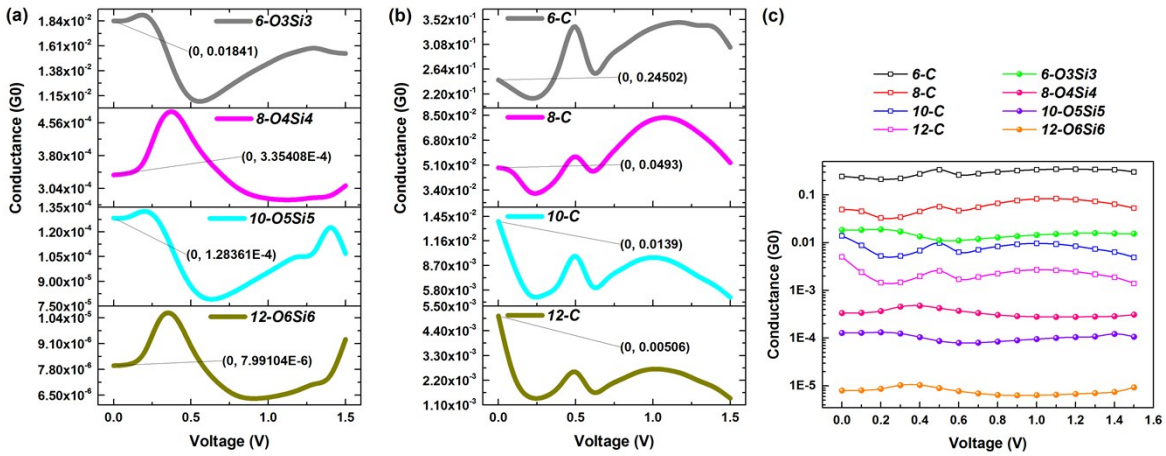

Figure S1 (a-b) Conductance versus voltage within the bias range [0V, 1.5V] for devices based on molecular siloxane rings and molecular alkane rings, respectively. Values of the equilibrium conductance have been displayed. (c) Comparison of conductance for all devices under the bias of [0V, 1.5V] on a log scale.

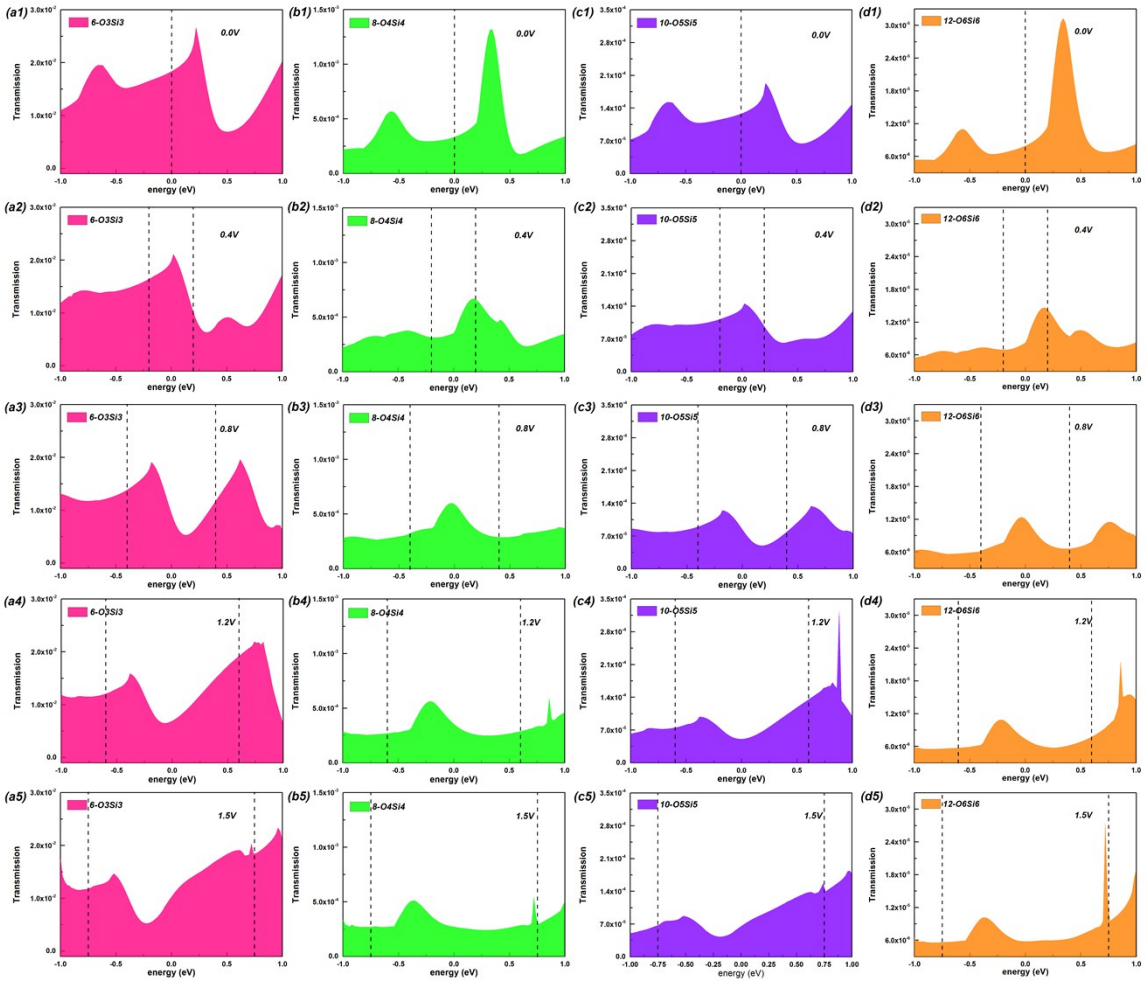

Figure S2 Transmission spectra in the energy region [-1eV, 1eV] at 0V, 0.4V, 0.8V, 1.2V and 1.5V for devices 6-O3Si3 (a1-a5), 8-O4Si4 (b1-b5), 10-O5Si5 (c1-c5) and 12-O6Si6 (d1-d5), respectively. The dotted lines indicate the bias window [-V/2, +V/2].

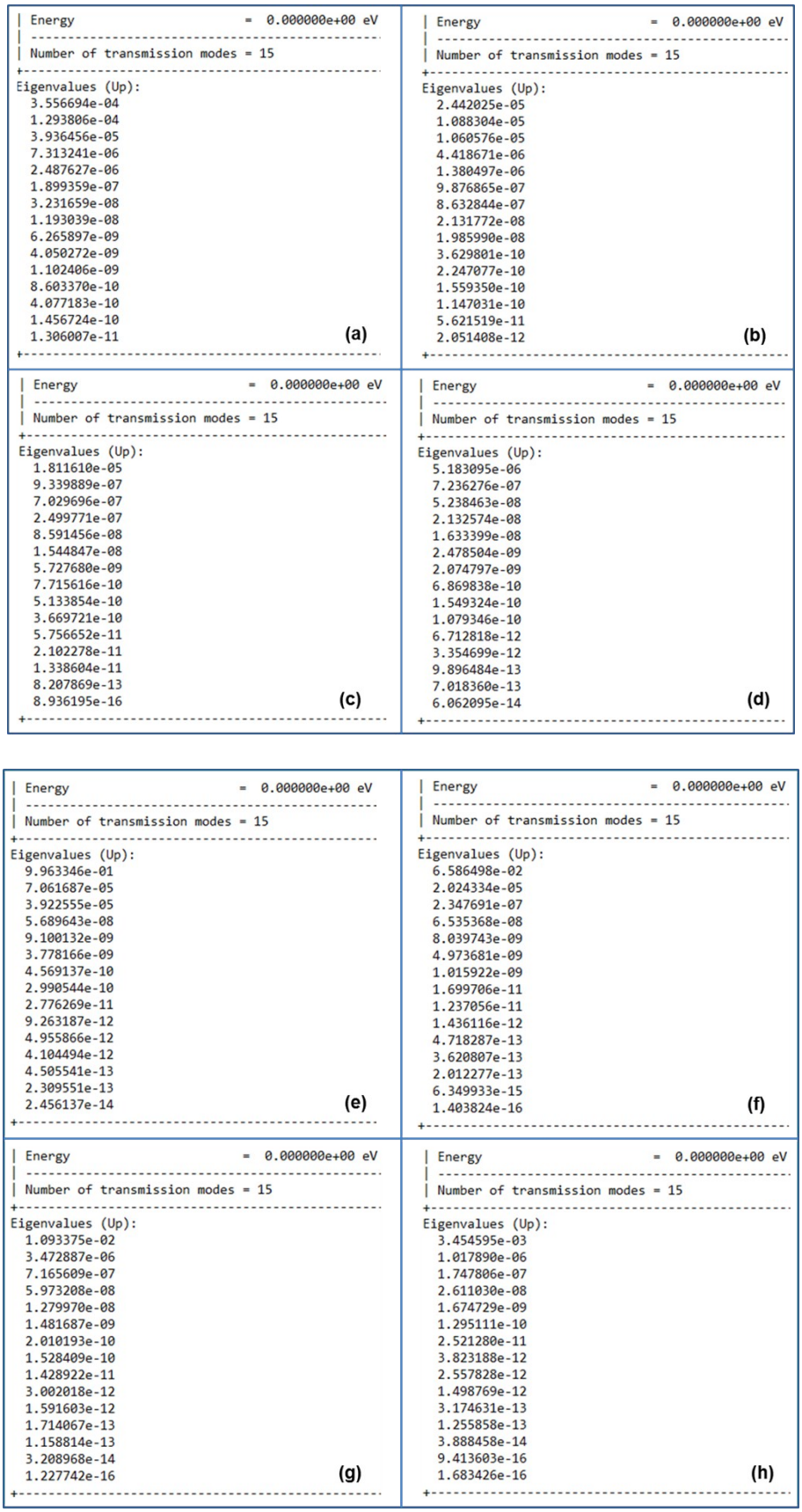

Figure S3 Transmission Reports of molecular siloxane rings-based devices (a-d) and molecular alkane rings-based devices (e-h).

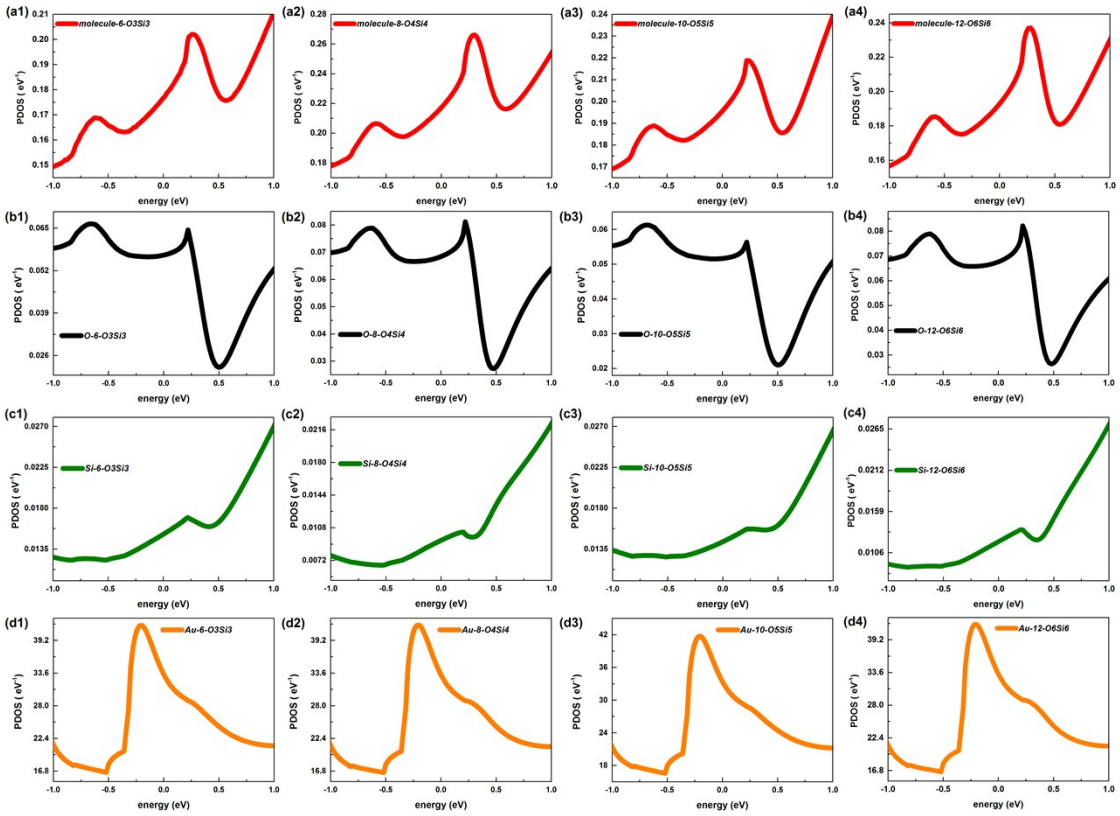

Figure S4 PDOS of molecular siloxane rings (a1)-(a4), PDOS of O atoms (b1)-(b4), PDOS of Si atoms (c1)-(c4) and PDOS of Au electrodes (d1)-(d4), for devices 6-O3Si3, 8-O4Si4, 10-O5Si5 and 12-O6Si6, respectively.

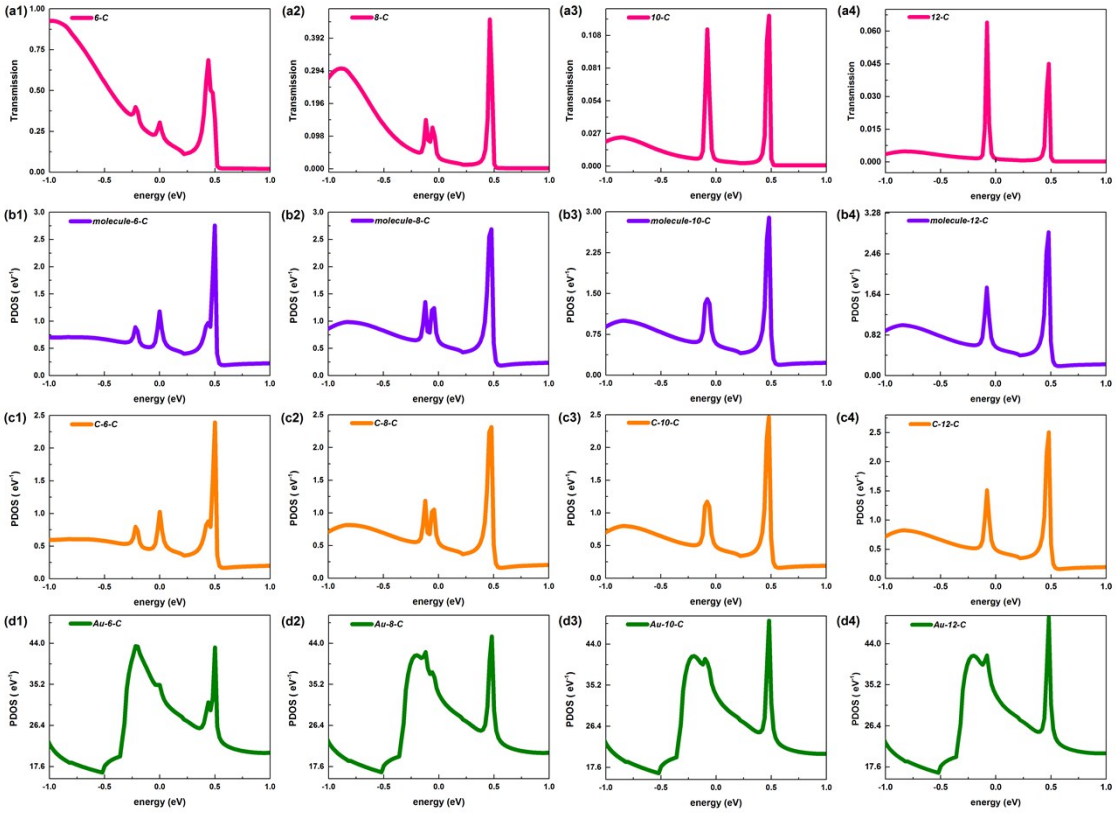

Figure S5 Equilibrium transmission spectra (a1)-(a4), PDOS of molecular alkane rings (b1)-(b4), PDOS of C atoms (c1)-(c4) and PDOS of Au electrodes (d1)-(d4), for devices 6-C, 8-C, 10-C and 12-C, respectively.

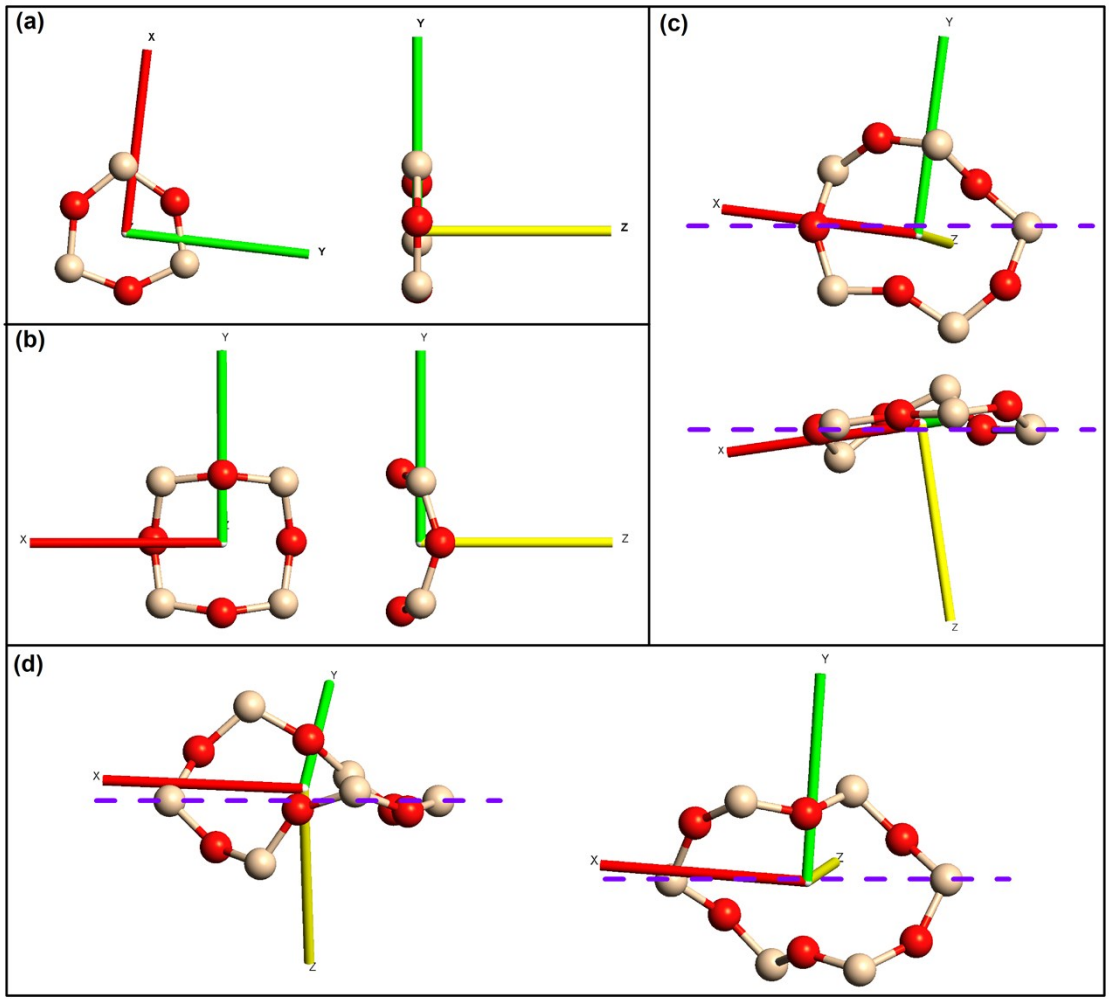

Figure S6 (a-d) Main rings displayed in different perspectives for 6-atoms siloxane ring, 8-atoms siloxane ring, 10-atoms siloxane ring and 12-atoms siloxane ring, respectively.

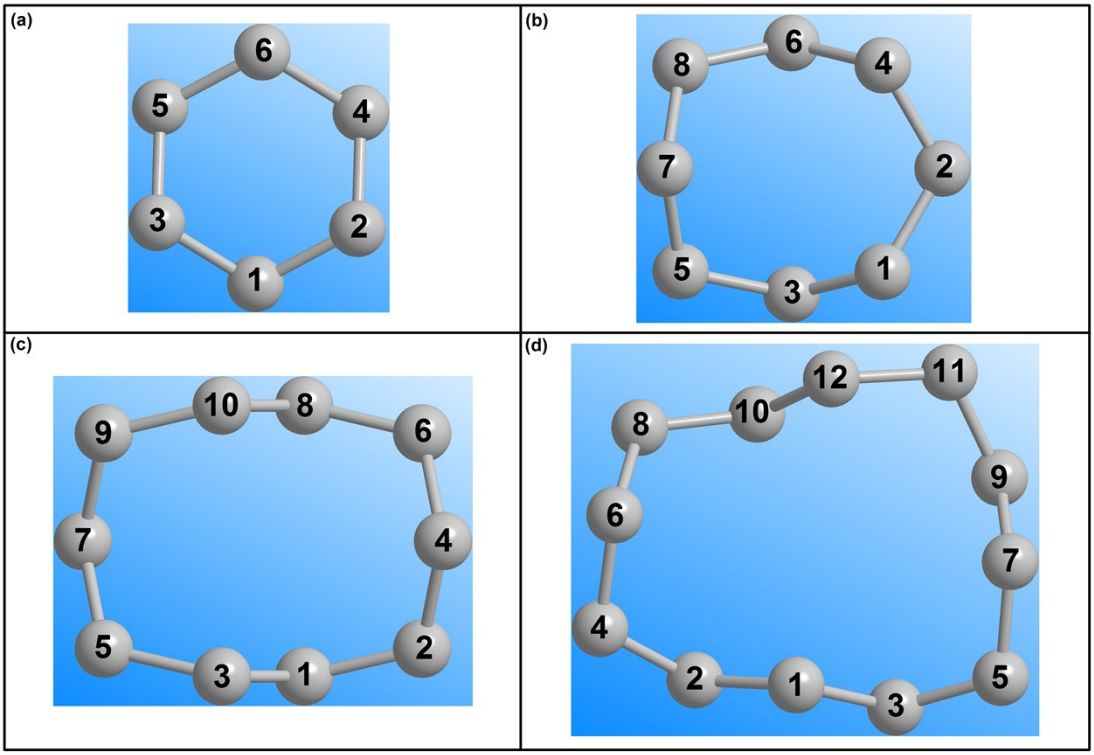

Figure S7 (a)-(d) Four main molecular alkane rings with atoms labeled with serial numbers. For clarity, the main rings are only shown, and C and H atoms have been hidden. These main molecular rings are respectively denoted by "C6", "C8", "C10" and "C12". For each molecular ring, the type of the dihedral angle is ranked clockwise from the atom labeled "1"one by one.

Table S1 Data of dihedral angles for all molecular alkane rings. The unit is the degree (°) for the dihedral angle and fluctuation degree.

Molecular Ring	NO.	Type of Dihedral Angle	Dihedral Angle	Deviation Value	Fluctuation Degree
C6	1	C(1)-C(3)-C(5)-C(6)	-54.269	54.269	0.0
	2	C(3)-C(5)-C(6)-C(4)	54.266	54.266	
	3	C(5)-C(6)-C(4)-C(2)	-54.261	54.261	
	4	C(6)-C(4)-C(2)-C(1)	54.259	54.259	
	5	C(4)-C(2)-C(1)-C(3)	-54.262	54.262	
	6	C(2)-C(1)-C(3)-C(5)	54.271	54.271	
C8	1	C(1)-C(3)-C(5)-C(7)	43.569	43.569	12.6
	2	C(3)-C(5)-C(7)-C(8)	64.332	64.332	
	3	C(5)-C(7)-C(8)-C(6)	-64.398	64.398	
	4	C(7)-C(8)-C(6)-C(4)	-43.472	43.472	
	5	C(8)-C(6)-C(4)-C(2)	77.774	77.774	
	6	C(6)-C(4)-C(2)-C(1)	-69.062	69.062	
	7	C(4)-C(2)-C(1)-C(3)	69.012	69.012	
	8	C(2)-C(1)-C(3)-C(5)	77.798	77.798	
C10	1	C(1)-C(3)-C(5)-C(7)	-55.073	55.073	13.9
	2	C(3)-C(5)-C(7)-C(9)	-66.042	66.042	
	3	C(5)-C(7)-C(9)-C(10)	65.993	65.993	
	4	C(7)-C(9)-C(10)-C(8)	55.134	55.134	
	5	C(9)-C(10)-C(8)-C(6)	28.121	28.121	
	6	C(10)-C(8)-C(6)-C(4)	55.108	55.108	
	7	C(8)-C(6)-C(4)-C(2)	66.008	66.008	
	8	C(6)-C(4)-C(2)-C(1)	-66.063	66.063	
	9	C(4)-C(2)-C(1)-C(3)	-55.045	55.045	
	10	C(2)-C(1)-C(3)-C(5)	28.158	28.158	
C12	1	C(1)-C(2)-C(4)-C(6)	56.763	56.763	23.6
	2	C(2)-C(4)-C(6)-C(8)	61.232	61.232	
	3	C(4)-C(6)-C(8)-C(10)	-83.728	83.728	
	4	C(6)-C(8)-C(10)-C(12)	-64.446	64.446	
	5	C(8)-C(10)-C(12)-C(11)	3.41	3.41	
	6	C(10)-C(12)-C(11)-C(9)	-61.301	61.301	
	7	C(12)-C(11)-C(9)-C(7)	-66.985	66.985	
	8	C(11)-C(9)-C(7)-C(5)	31.501	31.501	
	9	C(9)-C(7)-C(5)-C(3)	-59.504	59.504	
	10	C(7)-C(5)-C(3)-C(1)	-55.89	55.89	
	11	C(5)-C(3)-C(1)-C(2)	18.904	18.904	
	12	C(3)-C(1)-C(2)-C(4)	15.797	15.797	