Calculated Entropies for n-Heptane, 2-Methylhexane, 2,3- Dimethylpentane and Radicals from loss of H atoms

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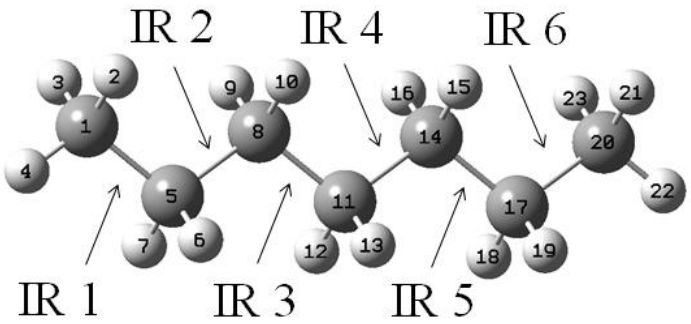
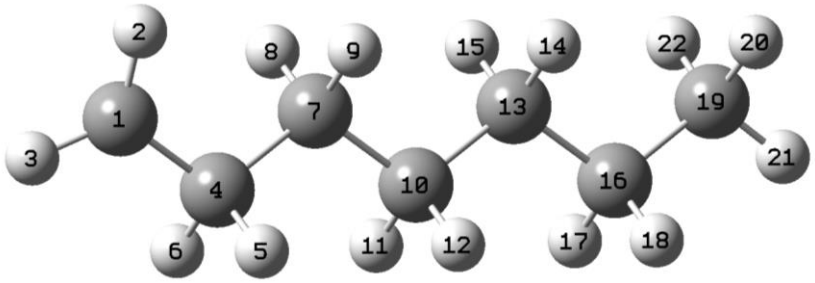
Supporting Information

Table S1: Geometry Parameters of *n*-c_7h_{16} Optimized at the B3LYP/6-31G(d,p) Level of Theory.



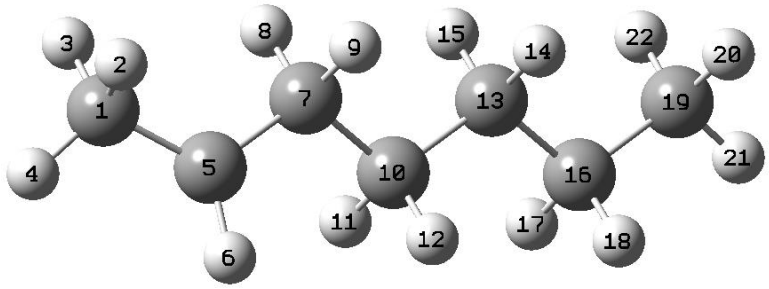
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
***n*-c_7h_{16}**										
σ = 18	R(1,2)	1.096	A(2,1,3)	107.45	A(16,14,17)	109.20	D(2,1,5,6)	62.291	D(8,11,14,17)	180.000
	R(1,3)	1.096	A(2,1,4)	107.65	A(14,17,18)	109.20	D(2,1,5,7)	178.032	D(12,11,14,15)	-179.983
	R(1,4)	1.095	A(2,1,5)	111.18	A(14,17,19)	109.20	D(2,1,5,8)	-59.838	D(12,11,14,16)	64.542
	R(1,5)	1.532	A(3,1,4)	107.65	A(14,17,20)	113.27	D(3,1,5,6)	-178.032	D(12,11,14,17)	-57.721
	R(5,6)	1.099	A(3,1,5)	111.18	A(18,17,19)	105.95	D(3,1,5,7)	-62.291	D(13,11,14,15)	-64.542
	R(5,7)	1.099	A(4,1,5)	111.52	A(18,17,20)	109.48	D(3,1,5,8)	59.838	D(13,11,14,16)	179.983
	R(5,8)	1.534	A(1,5,6)	109.48	A(19,17,20)	109.48	D(4,1,5,6)	-57.870	D(13,11,14,17)	57.720
	R(8,9)	1.100	A(1,5,7)	109.48	A(17,20,21)	111.18	D(4,1,5,7)	57.870	D(11,14,17,18)	57.714
	R(8,10)	1.100	A(1,5,8)	113.27	A(17,20,22)	111.52	D(4,1,5,8)	-180.000	D(11,14,17,19)	-57.714
	R(8,11)	1.533	A(6,5,7)	105.95	A(17,20,23)	111.18	D(1,5,8,9)	-57.679	D(11,14,17,20)	180.000
	R(11,12)	1.100	A(6,5,8)	109.20	A(21,20,22)	107.65	D(1,5,8,10)	57.679	D(15,14,17,18)	-179.965
	R(11,13)	1.100	A(7,5,8)	109.20	A(21,20,23)	107.45	D(1,5,8,11)	-180.000	D(15,14,17,19)	64.607
	R(11,14)	1.533	A(5,8,9)	109.20	A(22,20,23)	107.65	D(6,5,8,9)	-179.965	D(15,14,17,20)	-57.679
	R(14,15)	1.100	A(5,8,10)	109.20			D(6,5,8,10)	-64.607	D(16,14,17,18)	-64.607
	R(14,16)	1.100	A(5,8,11)	113.66			D(6,5,8,11)	57.714	D(16,14,17,19)	179.965
	R(14,17)	1.534	A(9,8,10)	105.89			D(7,5,8,9)	64.607	D(16,14,17,20)	57.679
	R(17,18)	1.099	A(9,8,11)	109.30			D(7,5,8,10)	179.965	D(14,17,20,21)	59.838
	R(17,19)	1.099	A(10,8,11)	109.30			D(7,5,8,11)	-57.714	D(14,17,20,22)	180.000
	R(17,20)	1.532	A(8,11,12)	109.25			D(5,8,11,12)	57.721	D(14,17,20,23)	-59.838
	R(20,21)	1.096	A(8,11,13)	109.25			D(5,8,11,13)	-57.720	D(18,17,20,21)	-178.032
	R(20,22)	1.095	A(8,11,14)	113.63			D(5,8,11,14)	-180.000	D(18,17,20,22)	-57.870
	R(20,23)	1.096	A(12,11,13)	105.91			D(9,8,11,12)	-64.542	D(18,17,20,23)	62.291
			A(12,11,14)	109.25			D(9,8,11,13)	-179.983	D(19,17,20,21)	-62.291
			A(13,11,14)	109.25			D(9,8,11,14)	57.738	D(19,17,20,22)	57.870
			A(11,14,15)	109.30			D(10,8,11,12)	179.983	D(19,17,20,23)	178.032
			A(11,14,16)	109.30			D(10,8,11,13)	64.542		
			A(11,14,17)	113.66			D(10,8,11,14)	-57.738		
			A(15,14,16)	105.89			D(8,11,14,15)	57.738		
			A(15,14,17)	109.20			D(8,11,14,16)	-57.738		

Table S2: Geometry Parameters of cjccccccc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



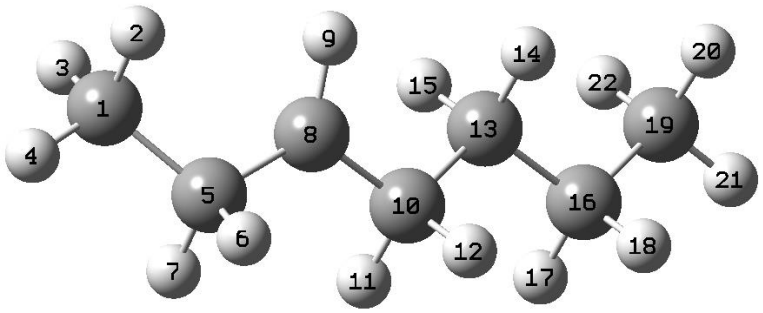
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cjccccccc										
σ = 3	R(1,2)	1.086	A(2,1,3)	117.57	A(13,16,19)	113.27	D(2,1,4,5)	90.149	D(11,10,13,16)	-57.675
	R(1,3)	1.085	A(2,1,4)	120.63	A(17,16,18)	105.96	D(2,1,4,6)	-155.068	D(12,10,13,14)	-64.444
	R(1,4)	1.491	A(3,1,4)	121.10	A(17,16,19)	109.47	D(2,1,4,7)	-31.637	D(12,10,13,15)	-179.945
	R(4,5)	1.107	A(1,4,5)	110.05	A(18,16,19)	109.48	D(3,1,4,5)	-80.051	D(12,10,13,16)	57.793
	R(4,6)	1.100	A(1,4,6)	109.87	A(16,19,20)	111.19	D(3,1,4,6)	34.732	D(10,13,16,17)	57.717
	R(4,7)	1.538	A(1,4,7)	113.87	A(16,19,21)	111.51	D(3,1,4,7)	158.164	D(10,13,16,18)	-57.726
	R(7,8)	1.098	A(5,4,6)	104.70	A(16,19,22)	111.19	D(1,4,7,8)	-58.889	D(10,13,16,19)	179.987
	R(7,9)	1.099	A(5,4,7)	108.28	A(20,19,21)	107.65	D(1,4,7,9)	56.496	D(14,13,16,17)	-179.989
	R(7,10)	1.533	A(6,4,7)	109.65	A(20,19,22)	107.46	D(1,4,7,10)	178.647	D(14,13,16,18)	64.568
	R(10,11)	1.100	A(4,7,8)	109.07	A(21,19,22)	107.65	D(5,4,7,8)	178.354	D(14,13,16,19)	-57.719
	R(10,12)	1.100	A(4,7,9)	108.97			D(5,4,7,9)	-66.261	D(15,13,16,17)	-64.597
	R(10,13)	1.533	A(4,7,10)	113.44			D(5,4,7,10)	55.890	D(15,13,16,18)	179.961
	R(13,14)	1.100	A(8,7,9)	106.08			D(6,4,7,8)	64.659	D(15,13,16,19)	57.674
	R(13,15)	1.100	A(8,7,10)	109.60			D(6,4,7,9)	-179.956	D(13,16,19,20)	59.739
	R(13,16)	1.534	A(9,7,10)	109.42			D(6,4,7,10)	-57.805	D(13,16,19,21)	179.895
	R(16,17)	1.099	A(7,10,11)	109.26			D(4,7,10,11)	57.927	D(13,16,19,22)	-59.952
	R(16,18)	1.099	A(7,10,12)	109.28			D(4,7,10,12)	-57.559	D(17,16,19,20)	-178.140
	R(16,19)	1.532	A(7,10,13)	113.56			D(4,7,10,13)	-179.853	D(17,16,19,21)	-57.984
	R(19,20)	1.096	A(11,10,12)	105.93			D(8,7,10,11)	-64.244	D(17,16,19,22)	62.169
	R(19,21)	1.095	A(11,10,13)	109.24			D(8,7,10,12)	-179.729	D(18,16,19,20)	-62.388
	R(19,22)	1.096	A(12,10,13)	109.28			D(8,7,10,13)	57.977	D(18,16,19,21)	57.768
			A(10,13,14)	109.30			D(9,7,10,11)	179.827	D(18,16,19,22)	177.921
			A(10,13,15)	109.31			D(9,7,10,12)	64.342		
			A(10,13,16)	113.62			D(9,7,10,13)	-57.953		
			A(14,13,15)	105.91			D(7,10,13,14)	57.851		
			A(14,13,16)	109.20			D(7,10,13,15)	-57.650		
			A(15,13,16)	109.21			D(7,10,13,16)	-179.911		
			A(13,16,17)	109.20			D(11,10,13,14)	-179.913		
			A(13,16,18)	109.20			D(11,10,13,15)	64.586		

Table S3: Geometry Parameters of ccjccccc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



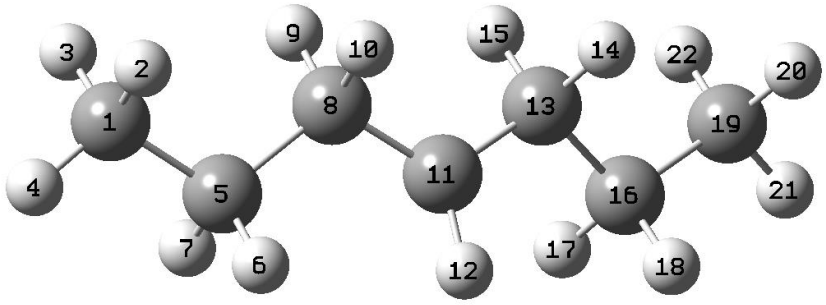
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
ccjccccc										
σ = 9	R(1,2)	1.105	A(2,1,3)	106.05	A(13,16,19)	113.28	D(2,1,5,6)	89.448	D(12,10,13,16)	57.827
	R(1,3)	1.098	A(2,1,4)	106.66	A(17,16,18)	105.97	D(2,1,5,7)	-75.018	D(10,13,16,17)	57.619
	R(1,4)	1.095	A(2,1,5)	112.25	A(17,16,19)	109.48	D(3,1,5,6)	-151.660	D(10,13,16,18)	-57.828
	R(1,5)	1.492	A(3,1,4)	108.02	A(18,16,19)	109.46	D(3,1,5,7)	43.874	D(10,13,16,19)	179.904
	R(5,6)	1.089	A(3,1,5)	111.58	A(16,19,20)	111.20	D(4,1,5,6)	-30.467	D(14,13,16,17)	179.963
	R(5,7)	1.494	A(4,1,5)	111.94	A(16,19,21)	111.50	D(4,1,5,7)	165.067	D(14,13,16,18)	64.516
	R(7,8)	1.102	A(1,5,6)	118.51	A(16,19,22)	111.19	D(1,5,7,8)	-42.758	D(14,13,16,19)	-57.752
	R(7,9)	1.108	A(1,5,7)	121.60	A(20,19,21)	107.65	D(1,5,7,9)	71.722	D(15,13,16,17)	-64.661
	R(7,10)	1.536	A(6,5,7)	118.10	A(20,19,22)	107.46	D(1,5,7,10)	-165.999	D(15,13,16,18)	179.892
	R(10,11)	1.098	A(5,7,8)	109.53	A(21,19,22)	107.65	D(6,5,7,8)	152.715	D(15,13,16,19)	57.624
	R(10,12)	1.099	A(5,7,9)	110.17			D(6,5,7,9)	-92.805	D(13,16,19,20)	59.914
	R(10,13)	1.533	A(5,7,10)	114.03			D(6,5,7,10)	29.474	D(13,16,19,21)	-179.936
	R(13,14)	1.100	A(8,7,9)	104.56			D(5,7,10,11)	58.302	D(13,16,19,22)	-59.787
	R(13,15)	1.100	A(8,7,10)	109.62			D(5,7,10,12)	-57.067	D(17,16,19,20)	-177.961
	R(13,16)	1.534	A(9,7,10)	108.51			D(5,7,10,13)	-179.215	D(17,16,19,21)	-57.811
	R(16,17)	1.099	A(7,10,11)	109.06			D(8,7,10,11)	-64.891	D(17,16,19,22)	62.338
	R(16,18)	1.099	A(7,10,12)	109.00			D(8,7,10,12)	179.741	D(18,16,19,20)	-62.214
	R(16,19)	1.532	A(7,10,13)	113.55			D(8,7,10,13)	57.593	D(18,16,19,21)	57.936
	R(19,20)	1.096	A(11,10,12)	106.06			D(9,7,10,11)	-178.513	D(18,16,19,22)	178.085
	R(19,21)	1.095	A(11,10,13)	109.56			D(9,7,10,12)	66.119		
	R(19,22)	1.096	A(12,10,13)	109.34			D(9,7,10,13)	-56.030		
			A(10,13,14)	109.33			D(7,10,13,14)	57.505		
			A(10,13,15)	109.32			D(7,10,13,15)	-58.015		
			A(10,13,16)	113.61			D(7,10,13,16)	179.787		
			A(14,13,15)	105.91			D(11,10,13,14)	179.710		
			A(14,13,16)	109.22			D(11,10,13,15)	64.190		
			A(15,13,16)	109.17			D(11,10,13,16)	-58.008		
			A(13,16,17)	109.19			D(12,10,13,14)	-64.455		
			A(13,16,18)	109.21			D(12,10,13,15)	-179.974		

Table S4: Geometry Parameters of cccjcccc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



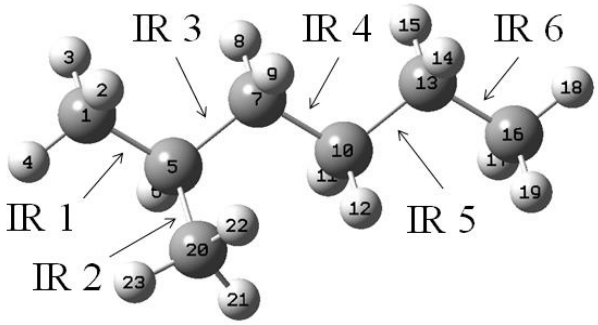
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cccjcccc										
σ = 9	R(1,2)	1.096	A(2,1,3)	107.60	A(13,16,19)	113.23	D(2,1,5,6)	64.157	D(12,10,13,16)	55.952
	R(1,3)	1.095	A(2,1,4)	107.71	A(17,16,18)	105.95	D(2,1,5,7)	178.025	D(10,13,16,17)	57.975
	R(1,4)	1.095	A(2,1,5)	110.94	A(17,16,19)	109.47	D(2,1,5,8)	-58.850	D(10,13,16,18)	-57.479
	R(1,5)	1.534	A(3,1,4)	108.04	A(18,16,19)	109.49	D(3,1,5,6)	-176.254	D(10,13,16,19)	-179.764
	R(5,6)	1.107	A(3,1,5)	111.01	A(16,19,20)	111.19	D(3,1,5,7)	-62.386	D(14,13,16,17)	-179.999
	R(5,7)	1.101	A(4,1,5)	111.38	A(16,19,21)	111.50	D(3,1,5,8)	60.739	D(14,13,16,18)	64.547
	R(5,8)	1.495	A(1,5,6)	108.64	A(16,19,22)	111.20	D(4,1,5,6)	-55.811	D(14,13,16,19)	-57.737
	R(8,9)	1.090	A(1,5,7)	109.78	A(20,19,21)	107.65	D(4,1,5,7)	58.057	D(15,13,16,17)	-64.263
	R(8,10)	1.494	A(1,5,8)	113.72	A(20,19,22)	107.46	D(4,1,5,8)	-178.818	D(15,13,16,18)	-179.717
	R(10,11)	1.101	A(6,5,7)	104.63	A(21,19,22)	107.65	D(1,5,8,9)	30.508	D(15,13,16,19)	57.999
	R(10,12)	1.108	A(6,5,8)	110.12			D(1,5,8,10)	-165.153	D(13,16,19,20)	59.926
	R(10,13)	1.536	A(7,5,8)	109.55			D(6,5,8,9)	-91.686	D(13,16,19,21)	-179.925
	R(13,14)	1.099	A(5,8,9)	118.02			D(6,5,8,10)	72.653	D(13,16,19,22)	-59.773
	R(13,15)	1.098	A(5,8,10)	122.07			D(7,5,8,9)	153.760	D(17,16,19,20)	-177.948
	R(13,16)	1.533	A(9,8,10)	118.09			D(7,5,8,10)	-41.901	D(17,16,19,21)	-57.799
	R(16,17)	1.099	A(8,10,11)	109.63			D(5,8,10,11)	42.227	D(17,16,19,22)	62.354
	R(16,18)	1.099	A(8,10,12)	110.21			D(5,8,10,12)	-72.367	D(18,16,19,20)	-62.209
	R(16,19)	1.532	A(8,10,13)	113.94			D(5,8,10,13)	165.441	D(18,16,19,21)	57.939
	R(19,20)	1.096	A(11,10,12)	104.58			D(9,8,10,11)	-153.446	D(18,16,19,22)	178.092
	R(19,21)	1.095	A(11,10,13)	109.58			D(9,8,10,12)	91.961		
	R(19,22)	1.096	A(12,10,13)	108.46			D(9,8,10,13)	-30.232		
			A(10,13,14)	109.06			D(8,10,13,14)	56.949		
			A(10,13,15)	109.10			D(8,10,13,15)	-58.439		
			A(10,13,16)	113.58			D(8,10,13,16)	179.101		
			A(14,13,15)	106.02			D(11,10,13,14)	-179.811		
			A(14,13,16)	109.29			D(11,10,13,15)	64.801		
			A(15,13,16)	109.51			D(11,10,13,16)	-57.659		
			A(13,16,17)	109.23			D(12,10,13,14)	-66.200		
			A(13,16,18)	109.22			D(12,10,13,15)	178.413		

Table S5: Geometry Parameters of ccccjccc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



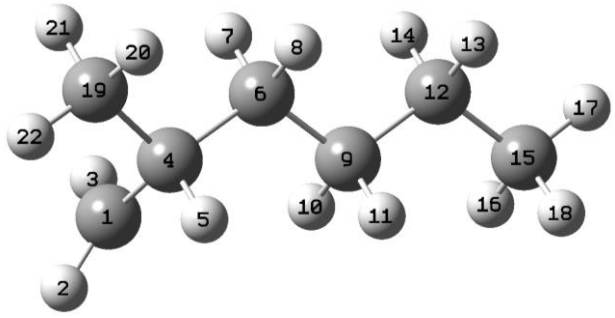
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
ccccjccc										
σ = 9	R(1,2)	1.096	A(2,1,3)	107.47	A(13,16,19)	113.23	D(2,1,5,6)	62.339	D(12,11,13,16)	31.720
	R(1,3)	1.096	A(2,1,4)	107.67	A(17,16,18)	106.08	D(2,1,5,7)	178.432	D(11,13,16,17)	58.319
	R(1,4)	1.095	A(2,1,5)	111.23	A(17,16,19)	109.77	D(2,1,5,8)	-59.500	D(11,13,16,18)	-57.033
	R(1,5)	1.531	A(3,1,4)	107.62	A(18,16,19)	109.53	D(3,1,5,6)	-177.899	D(11,13,16,19)	-179.189
	R(5,6)	1.098	A(3,1,5)	111.23	A(16,19,20)	111.23	D(3,1,5,7)	-61.805	D(14,13,16,17)	-178.500
	R(5,7)	1.097	A(4,1,5)	111.43	A(16,19,21)	111.43	D(3,1,5,8)	60.262	D(14,13,16,18)	66.149
	R(5,8)	1.537	A(1,5,6)	109.53	A(16,19,22)	111.23	D(4,1,5,6)	-57.811	D(14,13,16,19)	-56.008
	R(8,9)	1.101	A(1,5,7)	109.77	A(20,19,21)	107.67	D(4,1,5,7)	58.282	D(15,13,16,17)	-64.946
	R(8,10)	1.108	A(1,5,8)	113.23	A(20,19,22)	107.47	D(4,1,5,8)	-179.650	D(15,13,16,18)	179.702
	R(8,11)	1.494	A(6,5,7)	106.08	A(21,19,22)	107.62	D(1,5,8,9)	-57.546	D(15,13,16,19)	57.546
	R(11,12)	1.090	A(6,5,8)	108.96			D(1,5,8,10)	56.008	D(13,16,19,20)	59.500
	R(11,13)	1.494	A(7,5,8)	109.01			D(1,5,8,11)	179.189	D(13,16,19,21)	179.650
	R(13,14)	1.108	A(5,8,9)	109.54			D(6,5,8,9)	-179.702	D(13,16,19,22)	-60.262
	R(13,15)	1.101	A(5,8,10)	108.34			D(6,5,8,10)	-66.149	D(17,16,19,20)	-178.432
	R(13,16)	1.537	A(5,8,11)	114.03			D(6,5,8,11)	57.033	D(17,16,19,21)	-58.282
	R(16,17)	1.097	A(9,8,10)	104.61			D(7,5,8,9)	64.946	D(17,16,19,22)	61.805
	R(16,18)	1.098	A(9,8,11)	109.63			D(7,5,8,10)	178.500	D(18,16,19,20)	-62.339
	R(16,19)	1.531	A(10,8,11)	110.26			D(7,5,8,11)	-58.319	D(18,16,19,21)	57.811
	R(19,20)	1.096	A(8,11,12)	118.04			D(5,8,11,12)	-31.720	D(18,16,19,22)	177.899
	R(19,21)	1.095	A(8,11,13)	122.11			D(5,8,11,13)	163.955		
	R(19,22)	1.096	A(12,11,13)	118.04			D(9,8,11,12)	-154.933		
			A(11,13,14)	110.26			D(9,8,11,13)	40.741		
			A(11,13,15)	109.63			D(10,8,11,12)	90.414		
			A(11,13,16)	114.03			D(10,8,11,13)	-73.912		
			A(14,13,15)	104.61			D(8,11,13,14)	73.912		
			A(14,13,16)	108.34			D(8,11,13,15)	-40.741		
			A(15,13,16)	109.54			D(8,11,13,16)	-163.955		
			A(13,16,17)	109.01			D(12,11,13,14)	-90.414		
			A(13,16,18)	108.96			D(12,11,13,15)	154.933		

Table S6: Geometry Parameters of cc2cccc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



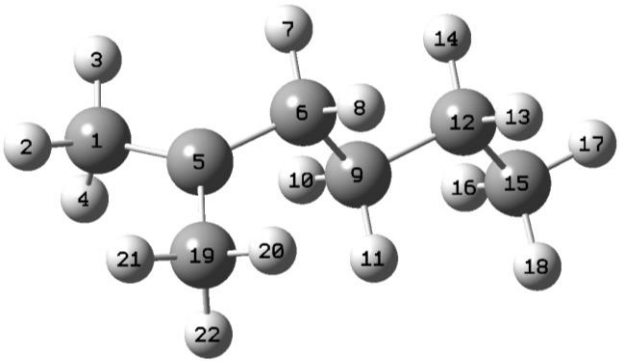
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2cccc										
σ = 27	R(1,2)	1.097	A(2,1,3)	107.60	A(15,13,16)	109.49	D(2,1,5,6)	-179.709	D(5,7,10,13)	175.572
	R(1,3)	1.096	A(2,1,4)	107.55	A(13,16,17)	111.19	D(2,1,5,7)	-62.486	D(8,7,10,11)	-68.182
	R(1,4)	1.095	A(2,1,5)	110.89	A(13,16,18)	111.51	D(2,1,5,20)	62.770	D(8,7,10,12)	175.710
	R(1,5)	1.536	A(3,1,4)	107.84	A(13,16,19)	111.20	D(3,1,5,6)	-59.866	D(8,7,10,13)	53.668
	R(5,6)	1.101	A(3,1,5)	111.44	A(17,16,18)	107.65	D(3,1,5,7)	57.357	D(9,7,10,11)	176.793
	R(5,7)	1.541	A(4,1,5)	111.34	A(17,16,19)	107.45	D(3,1,5,20)	-177.388	D(9,7,10,12)	60.686
	R(5,20)	1.536	A(1,5,6)	107.72	A(18,16,19)	107.64	D(4,1,5,6)	60.585	D(9,7,10,13)	-61.356
	R(7,8)	1.099	A(1,5,7)	110.53	A(5,20,21)	112.14	D(4,1,5,7)	177.808	D(7,10,13,14)	57.530
	R(7,9)	1.101	A(1,5,20)	110.49	A(5,20,22)	110.79	D(4,1,5,20)	-56.937	D(7,10,13,15)	-57.901
	R(7,10)	1.534	A(6,5,7)	107.54	A(5,20,23)	110.97	D(1,5,7,8)	-50.570	D(7,10,13,16)	179.787
	R(10,11)	1.100	A(6,5,20)	107.80	A(21,20,22)	107.72	D(1,5,7,9)	64.149	D(11,10,13,14)	179.472
	R(10,12)	1.098	A(7,5,20)	112.56	A(21,20,23)	107.49	D(1,5,7,10)	-172.528	D(11,10,13,15)	64.041
	R(10,13)	1.534	A(5,7,8)	108.43	A(22,20,23)	107.53	D(6,5,7,8)	66.765	D(11,10,13,16)	-58.271
	R(13,14)	1.099	A(5,7,9)	108.84			D(6,5,7,9)	-178.515	D(12,10,13,14)	-65.246
	R(13,15)	1.099	A(5,7,10)	115.43			D(6,5,7,10)	-55.192	D(12,10,13,15)	179.323
	R(13,16)	1.532	A(8,7,9)	105.87			D(20,5,7,8)	-174.650	D(12,10,13,16)	57.011
	R(16,17)	1.096	A(8,7,10)	108.53			D(20,5,7,9)	-59.930	D(10,13,16,17)	59.757
	R(16,18)	1.095	A(9,7,10)	109.32			D(20,5,7,10)	63.393	D(10,13,16,18)	179.908
	R(16,19)	1.096	A(7,10,11)	109.29			D(1,5,20,21)	175.767	D(10,13,16,19)	-59.941
	R(20,21)	1.094	A(7,10,12)	110.12			D(1,5,20,22)	-63.839	D(14,13,16,17)	-178.128
	R(20,22)	1.097	A(7,10,13)	113.20			D(1,5,20,23)	55.539	D(14,13,16,18)	-57.978
	R(20,23)	1.096	A(11,10,12)	106.04			D(6,5,20,21)	58.295	D(14,13,16,19)	62.173
			A(11,10,13)	109.13			D(6,5,20,22)	178.689	D(15,13,16,17)	-62.407
			A(12,10,13)	108.80			D(6,5,20,23)	-61.933	D(15,13,16,18)	57.744
			A(10,13,14)	109.20			D(7,5,20,21)	-60.135	D(15,13,16,19)	177.895
			A(10,13,15)	109.22			D(7,5,20,22)	60.259		
			A(10,13,16)	113.28			D(7,5,20,23)	179.637		
			A(14,13,15)	105.94			D(5,7,10,11)	53.722		
			A(14,13,16)	109.46			D(5,7,10,12)	-62.386		

Table S7: Geometry Parameters of cjc2cccc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



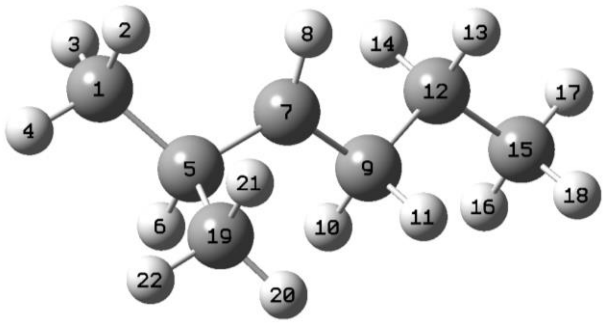
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cjc2cccc										
σ = 9	R(1,2)	1.086	A(2,1,3)	117.40	A(12,15,18)	111.19	D(2,1,4,5)	36.516	D(7,6,9,12)	57.074
O.I.	R(1,3)	1.087	A(2,1,4)	121.01	A(16,15,17)	107.67	D(2,1,4,6)	155.532	D(8,6,9,10)	178.889
	R(1,4)	1.497	A(3,1,4)	120.36	A(16,15,18)	107.44	D(2,1,4,19)	-80.378	D(8,6,9,11)	63.496
	R(4,5)	1.101	A(1,4,5)	108.29	A(17,15,18)	107.65	D(3,1,4,5)	-156.560	D(8,6,9,12)	-58.627
	R(4,6)	1.542	A(1,4,6)	112.13	A(4,19,20)	110.82	D(3,1,4,6)	-37.543	D(6,9,12,13)	57.436
	R(4,19)	1.550	A(1,4,19)	110.83	A(4,19,21)	110.74	D(3,1,4,19)	86.547	D(6,9,12,14)	-58.033
	R(6,7)	1.100	A(5,4,6)	107.96	A(4,19,22)	111.22	D(1,4,6,7)	58.767	D(6,9,12,15)	179.746
	R(6,8)	1.099	A(5,4,19)	106.85	A(20,19,21)	108.04	D(1,4,6,8)	173.841	D(10,9,12,13)	179.872
	R(6,9)	1.533	A(6,4,19)	110.57	A(20,19,22)	108.10	D(1,4,6,9)	-63.724	D(10,9,12,14)	64.404
	R(9,10)	1.098	A(4,6,7)	108.65	A(21,19,22)	107.79	D(5,4,6,7)	177.974	D(10,9,12,15)	-57.818
	R(9,11)	1.100	A(4,6,8)	108.95			D(5,4,6,8)	-66.953	D(11,9,12,13)	-64.649
	R(9,12)	1.533	A(4,6,9)	114.15			D(5,4,6,9)	55.482	D(11,9,12,14)	179.883
	R(12,13)	1.099	A(7,6,8)	106.01			D(19,4,6,7)	-65.472	D(11,9,12,15)	57.662
	R(12,14)	1.099	A(7,6,9)	109.49			D(19,4,6,8)	49.602	D(9,12,15,16)	59.648
	R(12,15)	1.532	A(8,6,9)	109.27			D(19,4,6,9)	172.037	D(9,12,15,17)	179.821
	R(15,16)	1.096	A(6,9,10)	109.34			D(1,4,19,20)	176.595	D(9,12,15,18)	-60.011
	R(15,17)	1.095	A(6,9,11)	109.17			D(1,4,19,21)	-63.518	D(13,12,15,16)	-178.117
	R(15,18)	1.096	A(6,9,12)	113.52			D(1,4,19,22)	56.322	D(13,12,15,17)	-57.944
	R(19,20)	1.096	A(10,9,11)	105.87			D(5,4,19,20)	58.819	D(13,12,15,18)	62.224
	R(19,21)	1.096	A(10,9,12)	109.42			D(5,4,19,21)	178.706	D(14,12,15,16)	-62.441
	R(19,22)	1.094	A(11,9,12)	109.24			D(5,4,19,22)	-61.454	D(14,12,15,17)	57.732
			A(9,12,13)	109.32			D(6,4,19,20)	-58.426	D(14,12,15,18)	177.899
			A(9,12,14)	109.21			D(6,4,19,21)	61.461		
			A(9,12,15)	113.24			D(6,4,19,22)	-178.699		
			A(13,12,14)	105.93			D(4,6,9,10)	56.624		
			A(13,12,15)	109.45			D(4,6,9,11)	-58.769		
			A(14,12,15)	109.44			D(4,6,9,12)	179.108		
			A(12,15,16)	111.17			D(7,6,9,10)	-65.410		
			A(12,15,17)	111.52			D(7,6,9,11)	179.196		

Table S8: Geometry Parameters of ccj2cccc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



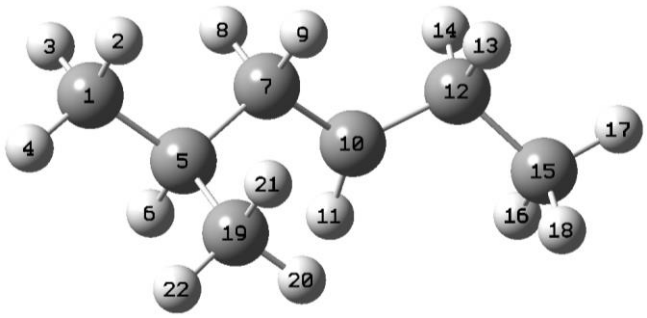
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
ccj2cccc										
σ = 54	R(1,2)	1.098	A(2,1,3)	108.05	A(12,15,18)	111.22	D(2,1,5,6)	-153.376	D(6,9,12,15)	180.000
	R(1,3)	1.096	A(2,1,4)	105.97	A(16,15,17)	107.64	D(2,1,5,19)	43.921	D(10,9,12,13)	179.722
	R(1,4)	1.105	A(2,1,5)	111.56	A(16,15,18)	107.45	D(3,1,5,6)	-32.253	D(10,9,12,14)	64.323
	R(1,5)	1.498	A(3,1,4)	106.60	A(17,15,18)	107.64	D(3,1,5,19)	165.044	D(10,9,12,15)	-57.977
	R(5,6)	1.501	A(3,1,5)	111.80	A(5,19,20)	111.80	D(4,1,5,6)	87.672	D(11,9,12,13)	-64.323
	R(5,19)	1.498	A(4,1,5)	112.51	A(5,19,21)	111.56	D(4,1,5,19)	-75.031	D(11,9,12,14)	-179.722
	R(6,7)	1.100	A(1,5,6)	119.62	A(5,19,22)	112.51	D(1,5,6,7)	40.415	D(11,9,12,15)	57.977
	R(6,8)	1.100	A(1,5,19)	118.45	A(20,19,21)	108.05	D(1,5,6,8)	157.089	D(9,12,15,16)	59.858
	R(6,9)	1.550	A(6,5,19)	119.62	A(20,19,22)	106.60	D(1,5,6,9)	-81.248	D(9,12,15,17)	-180.000
	R(9,10)	1.099	A(5,6,7)	109.70	A(21,19,22)	105.97	D(19,5,6,7)	-157.086	D(9,12,15,18)	-59.858
	R(9,11)	1.099	A(5,6,8)	109.70			D(19,5,6,8)	-40.412	D(13,12,15,16)	-178.020
	R(9,12)	1.533	A(5,6,9)	114.55			D(19,5,6,9)	81.251	D(13,12,15,17)	-57.879
	R(12,13)	1.099	A(7,6,8)	106.51			D(1,5,19,20)	-165.044	D(13,12,15,18)	62.263
	R(12,14)	1.099	A(7,6,9)	108.02			D(1,5,19,21)	-43.921	D(14,12,15,16)	-62.263
	R(12,15)	1.532	A(8,6,9)	108.02			D(1,5,19,22)	75.031	D(14,12,15,17)	57.879
	R(15,16)	1.096	A(6,9,10)	109.23			D(6,5,19,20)	32.253	D(14,12,15,18)	178.021
	R(15,17)	1.095	A(6,9,11)	109.23			D(6,5,19,21)	153.376		
	R(15,18)	1.096	A(6,9,12)	113.14			D(6,5,19,22)	-87.672		
	R(19,20)	1.096	A(10,9,11)	106.20			D(5,6,9,10)	57.883		
	R(19,21)	1.098	A(10,9,12)	109.40			D(5,6,9,11)	-57.883		
	R(19,22)	1.105	A(11,9,12)	109.40			D(5,6,9,12)	-180.000		
			A(9,12,13)	109.17			D(7,6,9,10)	-64.693		
			A(9,12,14)	109.17			D(7,6,9,11)	179.541		
			A(9,12,15)	113.30			D(7,6,9,12)	57.424		
			A(13,12,14)	105.95			D(8,6,9,10)	-179.541		
			A(13,12,15)	109.49			D(8,6,9,11)	64.694		
			A(14,12,15)	109.49			D(8,6,9,12)	-57.424		
			A(12,15,16)	111.22			D(6,9,12,13)	57.699		
			A(12,15,17)	111.49			D(6,9,12,14)	-57.699		

Table S9: Geometry Parameters of cc2cjccc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



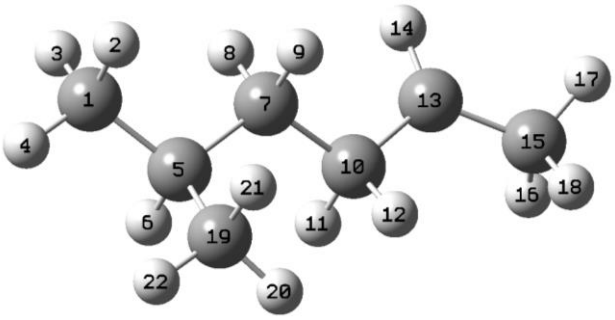
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2cjccc										
σ = 27	R(1,2)	1.097	A(2,1,3)	107.72	A(12,15,18)	111.24	D(2,1,5,6)	179.952	D(8,7,9,12)	-35.519
	R(1,3)	1.095	A(2,1,4)	107.62	A(16,15,17)	107.62	D(2,1,5,7)	-61.433	D(7,9,12,13)	56.648
	R(1,4)	1.095	A(2,1,5)	110.70	A(16,15,18)	107.46	D(2,1,5,19)	63.318	D(7,9,12,14)	-58.681
	R(1,5)	1.538	A(3,1,4)	108.16	A(17,15,18)	107.66	D(3,1,5,6)	-60.303	D(7,9,12,15)	178.805
	R(5,6)	1.101	A(3,1,5)	111.25	A(5,19,20)	111.40	D(3,1,5,7)	58.312	D(10,9,12,13)	179.838
	R(5,7)	1.501	A(4,1,5)	111.24	A(5,19,21)	110.68	D(3,1,5,19)	-176.936	D(10,9,12,14)	64.510
	R(5,19)	1.549	A(1,5,6)	108.13	A(5,19,22)	110.91	D(4,1,5,6)	60.350	D(10,9,12,15)	-58.005
	R(7,8)	1.091	A(1,5,7)	111.52	A(20,19,21)	107.85	D(4,1,5,7)	178.965	D(11,9,12,13)	-66.565
	R(7,9)	1.495	A(1,5,19)	110.46	A(20,19,22)	107.94	D(4,1,5,19)	-56.284	D(11,9,12,14)	178.107
	R(9,10)	1.101	A(6,5,7)	108.02	A(21,19,22)	107.93	D(1,5,7,8)	39.053	D(11,9,12,15)	55.593
	R(9,11)	1.108	A(6,5,19)	106.88			D(1,5,7,9)	-156.837	D(9,12,15,16)	59.995
	R(9,12)	1.538	A(7,5,19)	111.63			D(6,5,7,8)	157.735	D(9,12,15,17)	-179.907
	R(12,13)	1.098	A(5,7,8)	117.57			D(6,5,7,9)	-38.155	D(9,12,15,18)	-59.759
	R(12,14)	1.097	A(5,7,9)	122.76			D(19,5,7,8)	-85.047	D(13,12,15,16)	-178.193
	R(12,15)	1.531	A(8,7,9)	117.81			D(19,5,7,9)	79.063	D(13,12,15,17)	-58.095
	R(15,16)	1.096	A(7,9,10)	109.67			D(1,5,19,20)	178.190	D(13,12,15,18)	62.053
	R(15,17)	1.095	A(7,9,11)	110.53			D(1,5,19,21)	-61.821	D(14,12,15,16)	-62.066
	R(15,18)	1.096	A(7,9,12)	113.87			D(1,5,19,22)	57.938	D(14,12,15,17)	58.032
	R(19,20)	1.095	A(10,9,11)	104.78			D(6,5,19,20)	60.786	D(14,12,15,18)	178.180
	R(19,21)	1.096	A(10,9,12)	109.52			D(6,5,19,21)	-179.226		
	R(19,22)	1.096	A(11,9,12)	108.07			D(6,5,19,22)	-59.467		
			A(9,12,13)	108.94			D(7,5,19,20)	-57.116		
			A(9,12,14)	109.00			D(7,5,19,21)	62.872		
			A(9,12,15)	113.20			D(7,5,19,22)	-177.369		
			A(13,12,14)	106.08			D(5,7,9,10)	37.302		
			A(13,12,15)	109.56			D(5,7,9,11)	-77.728		
			A(14,12,15)	109.81			D(5,7,9,12)	160.407		
			A(12,15,16)	111.23			D(8,7,9,10)	-158.624		
			A(12,15,17)	111.44			D(8,7,9,11)	86.347		

Table S10: Geometry Parameters of cc2ccjcc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



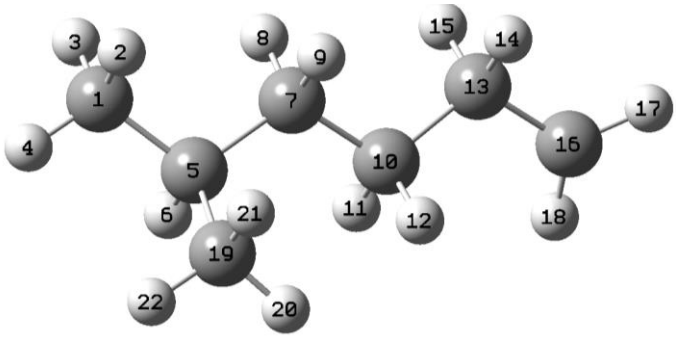
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2ccjcc										
σ = 27	R(1,2)	1.097	A(2,1,3)	107.65	A(12,15,18)	111.00	D(2,1,5,6)	-179.481	D(8,7,10,11)	-85.030
	R(1,3)	1.096	A(2,1,4)	107.52	A(16,15,17)	107.70	D(2,1,5,7)	-62.218	D(8,7,10,12)	78.080
	R(1,4)	1.095	A(2,1,5)	110.89	A(16,15,18)	107.61	D(2,1,5,19)	62.401	D(9,7,10,11)	160.171
	R(1,5)	1.534	A(3,1,4)	107.84	A(17,15,18)	108.04	D(3,1,5,6)	-59.552	D(9,7,10,12)	-36.720
	R(5,6)	1.101	A(3,1,5)	111.48	A(5,19,20)	111.30	D(3,1,5,7)	57.711	D(7,10,12,13)	42.045
	R(5,7)	1.544	A(4,1,5)	111.28	A(5,19,21)	110.66	D(3,1,5,19)	-177.670	D(7,10,12,14)	-72.526
	R(5,19)	1.535	A(1,5,6)	107.87	A(5,19,22)	111.31	D(4,1,5,6)	60.882	D(7,10,12,15)	165.306
	R(7,8)	1.108	A(1,5,7)	111.01	A(20,19,21)	107.60	D(4,1,5,7)	178.144	D(11,10,12,13)	-154.852
	R(7,9)	1.102	A(1,5,19)	111.07	A(20,19,22)	108.16	D(4,1,5,19)	-57.236	D(11,10,12,14)	90.578
	R(7,10)	1.495	A(6,5,7)	107.28	A(21,19,22)	107.65	D(1,5,7,8)	-49.180	D(11,10,12,15)	-31.590
	R(10,11)	1.091	A(6,5,19)	107.95			D(1,5,7,9)	64.348	D(10,12,15,16)	58.913
	R(10,12)	1.495	A(7,5,19)	111.47			D(1,5,7,10)	-172.039	D(10,12,15,17)	178.885
	R(12,13)	1.100	A(5,7,8)	108.08			D(6,5,7,8)	68.445	D(10,12,15,18)	-60.701
	R(12,14)	1.107	A(5,7,9)	109.20			D(6,5,7,9)	-178.027	D(13,12,15,16)	-177.970
	R(12,15)	1.534	A(5,7,10)	114.62			D(6,5,7,10)	-54.414	D(13,12,15,17)	-57.999
	R(15,16)	1.096	A(8,7,9)	104.85			D(19,5,7,8)	-173.575	D(13,12,15,18)	62.416
	R(15,17)	1.095	A(8,7,10)	109.85			D(19,5,7,9)	-60.047	D(14,12,15,16)	-64.089
	R(15,18)	1.095	A(9,7,10)	109.77			D(19,5,7,10)	63.565	D(14,12,15,17)	55.882
	R(19,20)	1.094	A(7,10,11)	117.80			D(1,5,19,20)	179.758	D(14,12,15,18)	176.297
	R(19,21)	1.097	A(7,10,12)	122.25			D(1,5,19,21)	-60.641		
	R(19,22)	1.095	A(11,10,12)	117.84			D(1,5,19,22)	59.015		
			A(10,12,13)	109.53			D(6,5,19,20)	61.690		
			A(10,12,14)	110.12			D(6,5,19,21)	-178.709		
			A(10,12,15)	113.74			D(6,5,19,22)	-59.053		
			A(13,12,14)	104.65			D(7,5,19,20)	-55.883		
			A(13,12,15)	109.79			D(7,5,19,21)	63.719		
			A(14,12,15)	108.61			D(7,5,19,22)	-176.626		
			A(12,15,16)	110.98			D(5,7,10,11)	36.867		
			A(12,15,17)	111.36			D(5,7,10,12)	-160.023		

Table S11: Geometry Parameters of cc2cccjc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



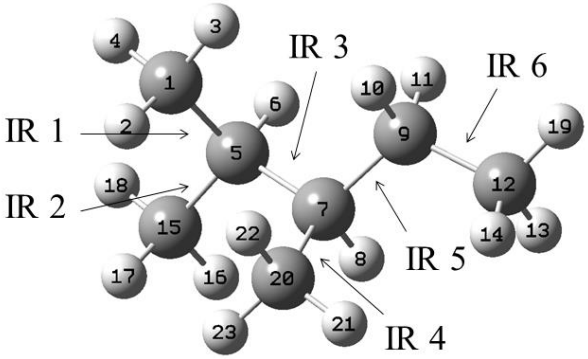
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2cccjc										
σ = 27	R(1,2)	1.097	A(2,1,3)	107.62	A(13,15,18)	111.60	D(2,1,5,6)	-179.900	D(5,7,10,13)	174.529
	R(1,3)	1.096	A(2,1,4)	107.54	A(16,15,17)	106.66	D(2,1,5,7)	-62.653	D(8,7,10,11)	-69.958
	R(1,4)	1.095	A(2,1,5)	110.89	A(16,15,18)	106.04	D(2,1,5,19)	62.551	D(8,7,10,12)	175.787
	R(1,5)	1.536	A(3,1,4)	107.84	A(17,15,18)	108.01	D(3,1,5,6)	-60.018	D(8,7,10,13)	52.773
	R(5,6)	1.101	A(3,1,5)	111.46	A(5,19,20)	112.17	D(3,1,5,7)	57.229	D(9,7,10,11)	175.089
	R(5,7)	1.541	A(4,1,5)	111.31	A(5,19,21)	110.77	D(3,1,5,19)	-177.567	D(9,7,10,12)	60.834
	R(5,19)	1.536	A(1,5,6)	107.75	A(5,19,22)	110.97	D(4,1,5,6)	60.419	D(9,7,10,13)	-62.180
	R(7,8)	1.099	A(1,5,7)	110.51	A(20,19,21)	107.71	D(4,1,5,7)	177.666	D(7,10,13,14)	-31.211
	R(7,9)	1.099	A(1,5,19)	110.48	A(20,19,22)	107.47	D(4,1,5,19)	-57.130	D(7,10,13,15)	164.274
	R(7,10)	1.538	A(6,5,7)	107.55	A(21,19,22)	107.56	D(1,5,7,8)	-50.782	D(11,10,13,14)	90.605
	R(10,11)	1.108	A(6,5,19)	107.82			D(1,5,7,9)	64.323	D(11,10,13,15)	-73.911
	R(10,12)	1.100	A(7,5,19)	112.53			D(1,5,7,10)	-172.404	D(12,10,13,14)	-154.916
	R(10,13)	1.495	A(5,7,8)	108.53			D(6,5,7,8)	66.589	D(12,10,13,15)	40.569
	R(13,14)	1.089	A(5,7,9)	109.19			D(6,5,7,9)	-178.307	D(10,13,15,16)	74.480
	R(13,15)	1.492	A(5,7,10)	115.29			D(6,5,7,10)	-55.034	D(10,13,15,17)	-165.608
	R(15,16)	1.105	A(8,7,9)	105.99			D(19,5,7,8)	-174.812	D(10,13,15,18)	-44.418
	R(15,17)	1.095	A(8,7,10)	108.28			D(19,5,7,9)	-59.708	D(14,13,15,16)	-89.971
	R(15,18)	1.098	A(9,7,10)	109.15			D(19,5,7,10)	63.565	D(14,13,15,17)	29.941
	R(19,20)	1.094	A(7,10,11)	108.44			D(1,5,19,20)	175.674	D(14,13,15,18)	151.132
	R(19,21)	1.097	A(7,10,12)	110.43			D(1,5,19,21)	-63.944		
	R(19,22)	1.095	A(7,10,13)	113.57			D(1,5,19,22)	55.454		
			A(11,10,12)	104.76			D(6,5,19,20)	58.166		
			A(11,10,13)	110.10			D(6,5,19,21)	178.548		
			A(12,10,13)	109.17			D(6,5,19,22)	-62.054		
			A(10,13,14)	118.05			D(7,5,19,20)	-60.278		
			A(10,13,15)	121.66			D(7,5,19,21)	60.104		
			A(14,13,15)	118.49			D(7,5,19,22)	179.502		
			A(13,15,16)	112.26			D(5,7,10,11)	51.798		
			A(13,15,17)	111.92			D(5,7,10,12)	-62.457		

Table S12: Geometry Parameters of cc2ccccj Optimized at the B3LYP/6-31G(d,p) Level of Theory.



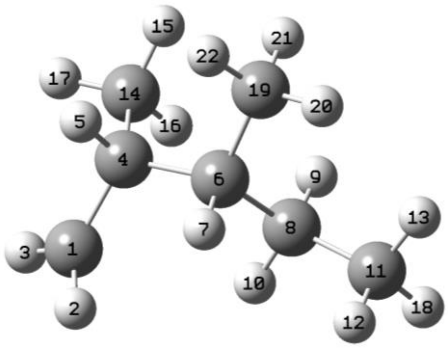
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2ccccj										
σ = 9	R(1,2)	1.097	A(2,1,3)	107.61	A(15,13,16)	110.06	D(2,1,5,6)	-179.575	D(5,7,10,13)	175.720
	R(1,3)	1.096	A(2,1,4)	107.56	A(13,16,17)	121.13	D(2,1,5,7)	-62.365	D(8,7,10,11)	-67.685
	R(1,4)	1.095	A(2,1,5)	110.90	A(13,16,18)	120.60	D(2,1,5,19)	62.864	D(8,7,10,12)	175.748
	R(1,5)	1.536	A(3,1,4)	107.84	A(17,16,18)	117.56	D(3,1,5,6)	-59.727	D(8,7,10,13)	53.808
	R(5,6)	1.101	A(3,1,5)	111.43	A(5,19,20)	112.14	D(3,1,5,7)	57.483	D(9,7,10,11)	177.254
	R(5,7)	1.541	A(4,1,5)	111.33	A(5,19,21)	110.78	D(3,1,5,19)	-177.288	D(9,7,10,12)	60.688
	R(5,19)	1.536	A(1,5,6)	107.72	A(5,19,22)	110.96	D(4,1,5,6)	60.711	D(9,7,10,13)	-61.253
	R(7,8)	1.099	A(1,5,7)	110.49	A(20,19,21)	107.72	D(4,1,5,7)	177.921	D(7,10,13,14)	57.848
	R(7,9)	1.101	A(1,5,19)	110.52	A(20,19,22)	107.50	D(4,1,5,19)	-56.850	D(7,10,13,15)	-55.876
	R(7,10)	1.534	A(6,5,7)	107.54	A(21,19,22)	107.53	D(1,5,7,8)	-50.309	D(7,10,13,16)	-178.634
	R(10,11)	1.099	A(6,5,19)	107.82			D(1,5,7,9)	64.443	D(11,10,13,14)	179.614
	R(10,12)	1.096	A(7,5,19)	112.54			D(1,5,7,10)	-172.256	D(11,10,13,15)	65.891
	R(10,13)	1.538	A(5,7,8)	108.47			D(6,5,7,8)	67.010	D(11,10,13,16)	-56.868
	R(13,14)	1.100	A(5,7,9)	108.83			D(6,5,7,9)	-178.239	D(12,10,13,14)	-65.099
	R(13,15)	1.107	A(5,7,10)	115.37			D(6,5,7,10)	-54.937	D(12,10,13,15)	-178.822
	R(13,16)	1.491	A(8,7,9)	105.88			D(19,5,7,8)	-174.384	D(12,10,13,16)	58.420
	R(16,17)	1.085	A(8,7,10)	108.53			D(19,5,7,9)	-59.633	D(10,13,16,17)	-157.488
	R(16,18)	1.086	A(9,7,10)	109.35			D(19,5,7,10)	63.669	D(10,13,16,18)	32.437
	R(19,20)	1.094	A(7,10,11)	109.39			D(1,5,19,20)	175.912	D(14,13,16,17)	-34.085
	R(19,21)	1.097	A(7,10,12)	110.45			D(1,5,19,21)	-63.692	D(14,13,16,18)	155.839
	R(19,22)	1.095	A(7,10,13)	113.00			D(1,5,19,22)	55.677	D(15,13,16,17)	80.725
			A(11,10,12)	106.22			D(6,5,19,20)	58.415	D(15,13,16,18)	-89.351
			A(11,10,13)	108.90			D(6,5,19,21)	178.811		
			A(12,10,13)	108.65			D(6,5,19,22)	-61.820		
			A(10,13,14)	109.65			D(7,5,19,20)	-60.027		
			A(10,13,15)	108.30			D(7,5,19,21)	60.369		
			A(10,13,16)	113.83			D(7,5,19,22)	179.738		
			A(14,13,15)	104.72			D(5,7,10,11)	54.227		
			A(14,13,16)	109.87			D(5,7,10,12)	-62.340		

Table S13: Geometry Parameters of cc2c2cc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



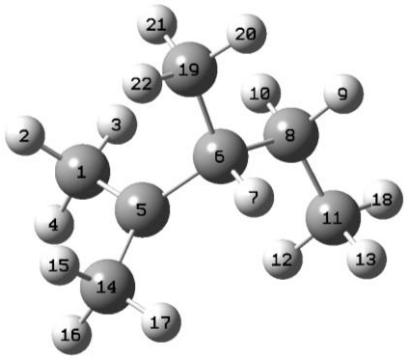
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2c2cc										
σ = 81	R(1,2)	1.096	A(2,1,3)	107.82	A(14,12,19)	107.27	D(2,1,5,6)	177.898	D(5,7,9,12)	-165.529
O.I.	R(1,3)	1.094	A(2,1,4)	107.23	A(5,15,16)	111.43	D(2,1,5,7)	-65.430	D(8,7,9,10)	-173.457
	R(1,4)	1.095	A(2,1,5)	111.58	A(5,15,17)	111.92	D(2,1,5,15)	62.001	D(8,7,9,11)	71.108
	R(1,5)	1.538	A(3,1,4)	107.43	A(5,15,18)	110.74	D(3,1,5,6)	-61.031	D(8,7,9,12)	-50.476
	R(5,6)	1.100	A(3,1,5)	112.12	A(16,15,17)	107.71	D(3,1,5,7)	55.642	D(20,7,9,10)	-56.561
	R(5,7)	1.556	A(4,1,5)	110.44	A(16,15,18)	107.69	D(3,1,5,15)	-176.928	D(20,7,9,11)	-171.997
	R(5,15)	1.537	A(1,5,6)	107.13	A(17,15,18)	107.14	D(4,1,5,6)	58.738	D(20,7,9,12)	66.420
	R(7,8)	1.101	A(1,5,7)	113.99	A(7,20,21)	111.19	D(4,1,5,7)	175.411	D(5,7,20,21)	172.697
	R(7,9)	1.544	A(1,5,15)	110.44	A(7,20,22)	111.46	D(4,1,5,15)	-57.159	D(5,7,20,22)	-67.570
	R(7,20)	1.538	A(6,5,7)	105.80	A(7,20,23)	111.81	D(1,5,7,8)	177.205	D(5,7,20,23)	53.112
	R(9,10)	1.098	A(6,5,15)	106.75	A(21,20,22)	107.34	D(1,5,7,9)	-67.188	D(8,7,20,21)	56.311
	R(9,11)	1.099	A(7,5,15)	112.23	A(21,20,23)	107.04	D(1,5,7,20)	59.933	D(8,7,20,22)	176.044
	R(9,12)	1.533	A(5,7,8)	105.76	A(22,20,23)	107.76	D(6,5,7,8)	-65.352	D(8,7,20,23)	-63.274
	R(12,13)	1.096	A(5,7,9)	111.59			D(6,5,7,9)	50.255	D(9,7,20,21)	-60.216
	R(12,14)	1.095	A(5,7,20)	113.38			D(6,5,7,20)	177.376	D(9,7,20,22)	59.518
	R(12,19)	1.095	A(8,7,9)	106.67			D(15,5,7,8)	50.704	D(9,7,20,23)	-179.800
	R(15,16)	1.096	A(8,7,20)	107.27			D(15,5,7,9)	166.311	D(7,9,12,13)	56.971
	R(15,17)	1.096	A(9,7,20)	111.65			D(15,5,7,20)	-66.568	D(7,9,12,14)	-63.499
	R(15,18)	1.096	A(7,9,10)	109.64			D(1,5,15,16)	179.194	D(7,9,12,19)	176.597
	R(20,21)	1.094	A(7,9,11)	108.59			D(1,5,15,17)	-60.131	D(10,9,12,13)	-179.720
	R(20,22)	1.096	A(7,9,12)	114.61			D(1,5,15,18)	59.347	D(10,9,12,14)	59.809
	R(20,23)	1.094	A(10,9,11)	106.03			D(6,5,15,16)	63.063	D(10,9,12,19)	-60.095
			A(10,9,12)	109.03			D(6,5,15,17)	-176.262	D(11,9,12,13)	-64.621
			A(11,9,12)	108.58			D(6,5,15,18)	-56.784	D(11,9,12,14)	174.909
			A(9,12,13)	111.15			D(7,5,15,16)	-52.414	D(11,9,12,19)	55.004
			A(9,12,14)	112.13			D(7,5,15,17)	68.261		
			A(9,12,19)	110.93			D(7,5,15,18)	-172.261		
			A(13,12,14)	107.59			D(5,7,9,10)	71.491		
			A(13,12,19)	107.56			D(5,7,9,11)	-43.945		

Table S14: Geometry Parameters of cjc2c2cc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



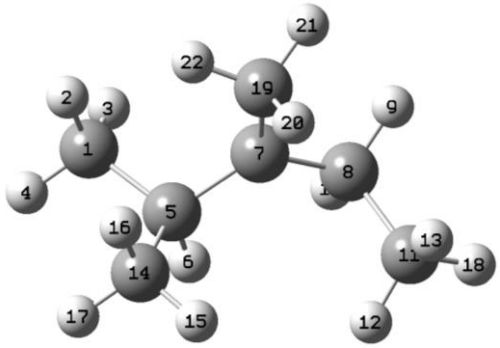
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cjc2c2cc										
σ = 27	R(1,2)	1.086	A(2,1,3)	117.54	A(4,14,17)	110.23	D(2,1,4,5)	-76.503	D(7,6,8,11)	-49.823
O.I.	R(1,3)	1.086	A(2,1,4)	120.59	A(15,14,16)	108.11	D(2,1,4,6)	38.355	D(19,6,8,9)	-55.330
	R(1,4)	1.495	A(3,1,4)	121.17	A(15,14,17)	107.46	D(2,1,4,14)	167.282	D(19,6,8,10)	-170.727
	R(4,5)	1.108	A(1,4,5)	107.55	A(16,14,17)	107.44	D(3,1,4,5)	93.649	D(19,6,8,11)	67.537
	R(4,6)	1.561	A(1,4,6)	111.62	A(6,19,20)	111.45	D(3,1,4,6)	-151.492	D(4,6,19,20)	171.376
	R(4,14)	1.540	A(1,4,14)	111.17	A(6,19,21)	111.65	D(3,1,4,14)	-22.565	D(4,6,19,21)	-68.614
	R(6,7)	1.101	A(5,4,6)	105.16	A(6,19,22)	111.13	D(1,4,6,7)	-50.004	D(4,6,19,22)	51.671
	R(6,8)	1.542	A(5,4,14)	106.49	A(20,19,21)	107.32	D(1,4,6,8)	66.393	D(7,6,19,20)	56.133
	R(6,19)	1.536	A(6,4,14)	114.31	A(20,19,22)	107.36	D(1,4,6,19)	-166.208	D(7,6,19,21)	176.143
	R(8,9)	1.098	A(4,6,7)	105.58	A(21,19,22)	107.71	D(5,4,6,7)	66.323	D(7,6,19,22)	-63.572
	R(8,10)	1.098	A(4,6,8)	112.39			D(5,4,6,8)	-177.280	D(8,6,19,20)	-61.178
	R(8,11)	1.533	A(4,6,19)	111.83			D(5,4,6,19)	-49.881	D(8,6,19,21)	58.832
	R(11,12)	1.096	A(7,6,8)	107.08			D(14,4,6,7)	-177.250	D(8,6,19,22)	179.117
	R(11,13)	1.095	A(7,6,19)	107.16			D(14,4,6,8)	-60.854	D(6,8,11,12)	57.373
	R(11,18)	1.095	A(8,6,19)	112.31			D(14,4,6,19)	66.545	D(6,8,11,13)	-63.054
	R(14,15)	1.094	A(6,8,9)	109.44			D(1,4,14,15)	176.623	D(6,8,11,18)	176.986
	R(14,16)	1.094	A(6,8,10)	108.40			D(1,4,14,16)	-62.150	D(9,8,11,12)	-179.620
	R(14,17)	1.095	A(6,8,11)	114.39			D(1,4,14,17)	57.095	D(9,8,11,13)	59.953
	R(19,20)	1.094	A(9,8,10)	106.18			D(5,4,14,15)	59.755	D(9,8,11,18)	-60.007
	R(19,21)	1.096	A(9,8,11)	109.19			D(5,4,14,16)	-179.018	D(10,8,11,12)	-64.076
	R(19,22)	1.096	A(10,8,11)	108.92			D(5,4,14,17)	-59.773	D(10,8,11,13)	175.497
			A(8,11,12)	111.12			D(6,4,14,15)	-55.899	D(10,8,11,18)	55.538
			A(8,11,13)	112.15			D(6,4,14,16)	65.328		
			A(8,11,18)	110.97			D(6,4,14,17)	-175.428		
			A(12,11,13)	107.56			D(4,6,8,9)	71.815		
			A(12,11,18)	107.55			D(4,6,8,10)	-43.582		
			A(13,11,18)	107.28			D(4,6,8,11)	-165.318		
			A(4,14,15)	111.90			D(7,6,8,9)	-172.690		
			A(4,14,16)	111.50			D(7,6,8,10)	71.913		

Table S15: Geometry Parameters of ccj2c2cc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



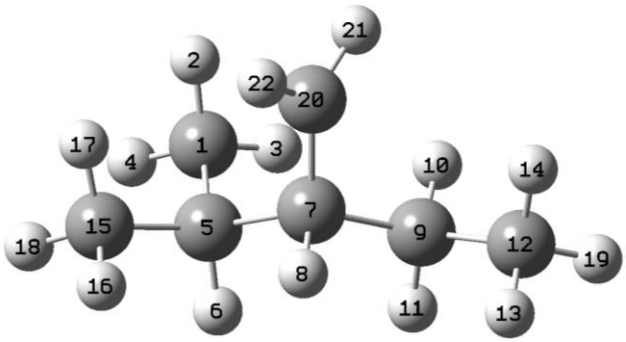
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
ccj2c2cc										
σ = 81	R(1,2)	1.105	A(2,1,3)	106.66	A(5,14,17)	111.92	D(2,1,5,6)	-91.534	D(5,6,19,22)	55.767
O.I.	R(1,3)	1.095	A(2,1,4)	105.98	A(15,14,16)	105.99	D(2,1,5,14)	70.206	D(7,6,19,20)	58.779
	R(1,4)	1.098	A(2,1,5)	112.10	A(15,14,17)	106.54	D(3,1,5,6)	28.796	D(7,6,19,21)	178.486
	R(1,5)	1.500	A(3,1,4)	107.74	A(16,14,17)	108.07	D(3,1,5,14)	-169.464	D(7,6,19,22)	-61.416
	R(5,6)	1.513	A(3,1,5)	112.68	A(6,19,20)	110.99	D(4,1,5,6)	149.960	D(8,6,19,20)	-57.039
	R(5,14)	1.498	A(4,1,5)	111.31	A(6,19,21)	111.07	D(4,1,5,14)	-48.300	D(8,6,19,21)	62.668
	R(6,7)	1.100	A(1,5,6)	120.33	A(6,19,22)	111.31	D(1,5,6,7)	179.800	D(8,6,19,22)	-177.234
	R(6,8)	1.547	A(1,5,14)	117.55	A(20,19,21)	107.64	D(1,5,6,8)	-62.500	D(6,8,11,12)	60.137
	R(6,19)	1.548	A(6,5,14)	119.55	A(20,19,22)	107.90	D(1,5,6,19)	62.722	D(6,8,11,13)	-59.528
	R(8,9)	1.098	A(5,6,7)	107.29	A(21,19,22)	107.77	D(14,5,6,7)	18.423	D(6,8,11,18)	-179.449
	R(8,10)	1.098	A(5,6,8)	113.43			D(14,5,6,8)	136.123	D(9,8,11,12)	-178.468
	R(8,11)	1.531	A(5,6,19)	111.65			D(14,5,6,19)	-98.655	D(9,8,11,13)	61.868
	R(11,12)	1.095	A(7,6,8)	106.80			D(1,5,14,15)	-77.513	D(9,8,11,18)	-58.053
	R(11,13)	1.096	A(7,6,19)	107.12			D(1,5,14,16)	41.392	D(10,8,11,12)	-62.913
	R(11,18)	1.095	A(8,6,19)	110.19			D(1,5,14,17)	162.688	D(10,8,11,13)	177.423
	R(14,15)	1.106	A(6,8,9)	108.27			D(6,5,14,15)	84.374	D(10,8,11,18)	57.501
	R(14,16)	1.097	A(6,8,10)	109.45			D(6,5,14,16)	-156.721		
	R(14,17)	1.096	A(6,8,11)	113.97			D(6,5,14,17)	-35.425		
	R(19,20)	1.096	A(9,8,10)	105.73			D(5,6,8,9)	177.537		
	R(19,21)	1.096	A(9,8,11)	109.47			D(5,6,8,10)	62.741		
	R(19,22)	1.095	A(10,8,11)	109.62			D(5,6,8,11)	-60.402		
			A(8,11,12)	111.21			D(7,6,8,9)	-64.481		
			A(8,11,13)	111.12			D(7,6,8,10)	-179.277		
			A(8,11,18)	111.30			D(7,6,8,11)	57.580		
			A(12,11,13)	107.46			D(19,6,8,9)	51.533		
			A(12,11,18)	107.96			D(19,6,8,10)	-63.263		
			A(13,11,18)	107.62			D(19,6,8,11)	173.594		
			A(5,14,15)	112.32			D(5,6,19,20)	175.962		
			A(5,14,16)	111.65			D(5,6,19,21)	-64.331		

Table S16: Geometry Parameters of cc2cj2cc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



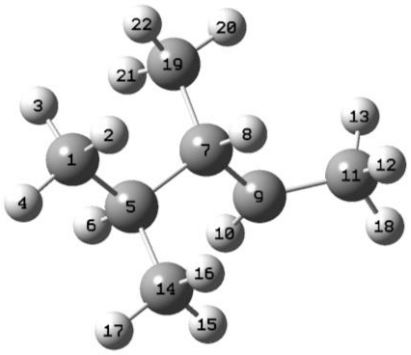
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2cj2cc										
σ = 81	R(1,2)	1.096	A(2,1,3)	107.75	A(5,14,17)	110.87	D(2,1,5,6)	179.771	D(19,7,8,11)	86.388
	R(1,3)	1.094	A(2,1,4)	107.54	A(15,14,16)	107.72	D(2,1,5,7)	-62.856	D(5,7,19,20)	92.442
	R(1,4)	1.096	A(2,1,5)	111.14	A(15,14,17)	108.00	D(2,1,5,14)	63.481	D(5,7,19,21)	-148.435
	R(1,5)	1.546	A(3,1,4)	108.12	A(16,14,17)	107.49	D(3,1,5,6)	-60.185	D(5,7,19,22)	-27.602
	R(5,6)	1.099	A(3,1,5)	111.21	A(7,19,20)	112.71	D(3,1,5,7)	57.188	D(8,7,19,20)	-77.889
	R(5,7)	1.513	A(4,1,5)	110.92	A(7,19,21)	111.34	D(3,1,5,14)	-176.475	D(8,7,19,21)	41.234
	R(5,14)	1.545	A(1,5,6)	107.06	A(7,19,22)	112.32	D(4,1,5,6)	60.184	D(8,7,19,22)	162.067
	R(7,8)	1.502	A(1,5,7)	111.83	A(20,19,21)	106.12	D(4,1,5,7)	177.557	D(7,8,11,12)	60.287
	R(7,19)	1.499	A(1,5,14)	110.17	A(20,19,22)	106.30	D(4,1,5,14)	-56.106	D(7,8,11,13)	-59.695
	R(8,9)	1.099	A(6,5,7)	107.40	A(21,19,22)	107.66	D(1,5,7,8)	-118.476	D(7,8,11,18)	-179.758
	R(8,10)	1.099	A(6,5,14)	107.24			D(1,5,7,19)	71.268	D(9,8,11,12)	-177.093
	R(8,11)	1.548	A(7,5,14)	112.83			D(6,5,7,8)	-1.306	D(9,8,11,13)	62.925
	R(11,12)	1.095	A(5,7,8)	119.86			D(6,5,7,19)	-171.563	D(9,8,11,18)	-57.138
	R(11,13)	1.095	A(5,7,19)	120.34			D(14,5,7,8)	116.653	D(10,8,11,12)	-62.152
	R(11,18)	1.096	A(8,7,19)	119.09			D(14,5,7,19)	-53.604	D(10,8,11,13)	177.866
	R(14,15)	1.095	A(7,8,9)	109.82			D(1,5,14,15)	176.709	D(10,8,11,18)	57.803
	R(14,16)	1.096	A(7,8,10)	109.75			D(1,5,14,16)	-63.119		
	R(14,17)	1.096	A(7,8,11)	114.13			D(1,5,14,17)	56.407		
	R(19,20)	1.104	A(9,8,10)	106.44			D(6,5,14,15)	60.532		
	R(19,21)	1.098	A(9,8,11)	108.26			D(6,5,14,16)	-179.296		
	R(19,22)	1.096	A(10,8,11)	108.13			D(6,5,14,17)	-59.770		
			A(8,11,12)	111.11			D(7,5,14,15)	-57.521		
			A(8,11,13)	111.15			D(7,5,14,16)	62.652		
			A(8,11,18)	111.01			D(7,5,14,17)	-177.822		
			A(12,11,13)	107.75			D(5,7,8,9)	154.241		
			A(12,11,18)	107.80			D(5,7,8,10)	37.555		
			A(13,11,18)	107.86			D(5,7,8,11)	-83.991		
			A(5,14,15)	111.39			D(19,7,8,9)	-35.380		
			A(5,14,16)	111.19			D(19,7,8,10)	-152.066		

Table S17: Geometry Parameters of cc2c2jcc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



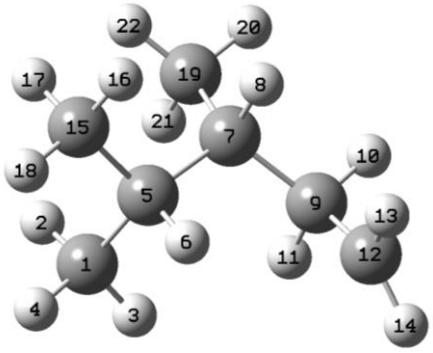
Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2c2jcc										
σ = 27	R(1,2)	1.096	A(2,1,3)	107.86	A(14,12,19)	107.89	D(2,1,5,6)	-179.196	D(5,7,9,12)	-165.880
O.I.	R(1,3)	1.094	A(2,1,4)	107.63	A(5,15,16)	111.46	D(2,1,5,7)	-62.525	D(8,7,9,10)	-173.628
	R(1,4)	1.095	A(2,1,5)	110.99	A(5,15,17)	111.21	D(2,1,5,15)	63.423	D(8,7,9,11)	70.632
	R(1,5)	1.536	A(3,1,4)	107.45	A(5,15,18)	110.87	D(3,1,5,6)	-58.471	D(8,7,9,12)	-51.448
	R(5,6)	1.100	A(3,1,5)	112.16	A(16,15,17)	107.81	D(3,1,5,7)	58.201	D(20,7,9,10)	-55.863
	R(5,7)	1.570	A(4,1,5)	110.56	A(16,15,18)	107.73	D(3,1,5,15)	-175.851	D(20,7,9,11)	-171.602
	R(5,15)	1.535	A(1,5,6)	107.83	A(17,15,18)	107.58	D(4,1,5,6)	61.437	D(20,7,9,12)	66.318
	R(7,8)	1.102	A(1,5,7)	113.23	A(7,20,21)	120.85	D(4,1,5,7)	178.108	D(5,7,20,21)	-93.658
	R(7,9)	1.544	A(1,5,15)	110.70	A(7,20,22)	121.56	D(4,1,5,15)	-55.944	D(5,7,20,22)	79.999
	R(7,20)	1.496	A(6,5,7)	105.78	A(21,20,22)	117.30	D(1,5,7,8)	179.294	D(8,7,20,21)	150.826
	R(9,10)	1.098	A(6,5,15)	107.54			D(1,5,7,9)	-64.854	D(8,7,20,22)	-35.517
	R(9,11)	1.098	A(7,5,15)	111.42			D(1,5,7,20)	62.076	D(9,7,20,21)	33.401
	R(9,12)	1.532	A(5,7,8)	104.90			D(6,5,7,8)	-62.830	D(9,7,20,22)	-152.942
	R(12,13)	1.096	A(5,7,9)	111.78			D(6,5,7,9)	53.023	D(7,9,12,13)	60.606
	R(12,14)	1.095	A(5,7,20)	113.16			D(6,5,7,20)	179.952	D(7,9,12,14)	-59.065
	R(12,19)	1.095	A(8,7,9)	107.21			D(15,5,7,8)	53.733	D(7,9,12,19)	-179.411
	R(15,16)	1.096	A(8,7,20)	107.78			D(15,5,7,9)	169.585	D(10,9,12,13)	-177.114
	R(15,17)	1.096	A(9,7,20)	111.54			D(15,5,7,20)	-63.486	D(10,9,12,14)	63.216
	R(15,18)	1.095	A(7,9,10)	109.39			D(1,5,15,16)	178.714	D(10,9,12,19)	-57.131
	R(20,21)	1.086	A(7,9,11)	109.01			D(1,5,15,17)	-60.953	D(11,9,12,13)	-61.288
	R(20,22)	1.085	A(7,9,12)	113.41			D(1,5,15,18)	58.704	D(11,9,12,14)	179.042
			A(10,9,11)	106.21			D(6,5,15,16)	61.151	D(11,9,12,19)	58.695
			A(10,9,12)	109.21			D(6,5,15,17)	-178.517		
			A(11,9,12)	109.35			D(6,5,15,18)	-58.859		
			A(9,12,13)	111.10			D(7,5,15,16)	-54.334		
			A(9,12,14)	111.25			D(7,5,15,17)	65.999		
			A(9,12,19)	111.30			D(7,5,15,18)	-174.344		
			A(13,12,14)	107.46			D(5,7,9,10)	71.940		
			A(13,12,19)	107.68			D(5,7,9,11)	-43.800		

Table S18: Geometry Parameters of cc2c2cjc Optimized at the B3LYP/6-31G(d,p) Level of Theory.



Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2c2cjc										
σ = 81	R(1,2)	1.097	A(2,1,3)	107.83	A(5,14,17)	111.09	D(2,1,5,6)	-175.514	D(8,7,9,10)	161.865
O.I.	R(1,3)	1.093	A(2,1,4)	107.38	A(15,14,16)	107.60	D(2,1,5,7)	-57.552	D(8,7,9,11)	-35.486
	R(1,4)	1.095	A(2,1,5)	110.94	A(15,14,17)	108.19	D(2,1,5,14)	67.075	D(19,7,9,10)	-81.615
	R(1,5)	1.536	A(3,1,4)	107.38	A(16,14,17)	107.55	D(3,1,5,6)	-54.584	D(19,7,9,11)	81.034
	R(5,6)	1.102	A(3,1,5)	112.55	A(7,19,20)	110.67	D(3,1,5,7)	63.378	D(5,7,19,20)	-176.767
	R(5,7)	1.554	A(4,1,5)	110.53	A(7,19,21)	110.77	D(3,1,5,14)	-171.995	D(5,7,19,21)	-57.447
	R(5,14)	1.537	A(1,5,6)	107.78	A(7,19,22)	112.00	D(4,1,5,6)	65.474	D(5,7,19,22)	63.321
	R(7,8)	1.103	A(1,5,7)	113.04	A(20,19,21)	107.65	D(4,1,5,7)	-176.564	D(8,7,19,20)	65.425
	R(7,9)	1.503	A(1,5,14)	109.92	A(20,19,22)	107.48	D(4,1,5,14)	-51.937	D(8,7,19,21)	-175.256
	R(7,19)	1.551	A(6,5,7)	106.94	A(21,19,22)	108.09	D(1,5,7,8)	64.832	D(8,7,19,22)	-54.487
	R(9,10)	1.090	A(6,5,14)	107.94			D(1,5,7,9)	-176.883	D(9,7,19,20)	-51.747
	R(9,11)	1.492	A(7,5,14)	110.99			D(1,5,7,19)	-52.745	D(9,7,19,21)	67.573
	R(11,12)	1.098	A(5,7,8)	107.43			D(6,5,7,8)	-176.715	D(9,7,19,22)	-171.659
	R(11,13)	1.105	A(5,7,9)	111.55			D(6,5,7,9)	-58.430	D(7,9,11,12)	42.704
	R(11,18)	1.095	A(5,7,19)	112.54			D(6,5,7,19)	65.708	D(7,9,11,13)	-76.554
	R(14,15)	1.094	A(8,7,9)	108.08			D(14,5,7,8)	-59.212	D(7,9,11,18)	163.799
	R(14,16)	1.097	A(8,7,19)	107.04			D(14,5,7,9)	59.073	D(10,9,11,12)	-154.773
	R(14,17)	1.095	A(9,7,19)	109.95			D(14,5,7,19)	-176.789	D(10,9,11,13)	85.969
	R(19,20)	1.095	A(7,9,10)	117.35			D(1,5,14,15)	178.668	D(10,9,11,18)	-33.678
	R(19,21)	1.096	A(7,9,11)	122.30			D(1,5,14,16)	-61.550		
	R(19,22)	1.094	A(10,9,11)	118.11			D(1,5,14,17)	57.841		
			A(9,11,12)	111.58			D(6,5,14,15)	61.357		
			A(9,11,13)	112.54			D(6,5,14,16)	-178.861		
			A(9,11,18)	111.77			D(6,5,14,17)	-59.470		
			A(12,11,13)	106.19			D(7,5,14,15)	-55.532		
			A(12,11,18)	108.04			D(7,5,14,16)	64.250		
			A(13,11,18)	106.39			D(7,5,14,17)	-176.359		
			A(5,14,15)	111.59			D(5,7,9,10)	43.971		
			A(5,14,16)	110.65			D(5,7,9,11)	-153.379		

Table S19: Geometry Parameters of cc2c2ccj Optimized at the B3LYP/6-31G(d,p) Level of Theory.



Species	Bond Distances (Angstroms)		Angles (Degrees)				Dihedral Angles (Degrees)			
cc2c2ccj										
σ = 27	R(1,2)	1.096	A(2,1,3)	107.80	A(5,15,18)	110.82	D(2,1,5,6)	176.912	D(5,7,9,12)	-61.232
O.I.	R(1,3)	1.095	A(2,1,4)	107.27	A(16,15,17)	107.69	D(2,1,5,7)	-66.493	D(8,7,9,10)	-67.382
	R(1,4)	1.095	A(2,1,5)	111.65	A(16,15,18)	107.68	D(2,1,5,15)	60.505	D(8,7,9,11)	179.200
	R(1,5)	1.537	A(3,1,4)	107.31	A(17,15,18)	107.14	D(3,1,5,6)	-61.941	D(8,7,9,12)	54.490
	R(5,6)	1.099	A(3,1,5)	112.20	A(7,19,20)	110.59	D(3,1,5,7)	54.655	D(19,7,9,10)	48.746
	R(5,7)	1.555	A(4,1,5)	110.38	A(7,19,21)	111.57	D(3,1,5,15)	-178.348	D(19,7,9,11)	-64.672
	R(5,15)	1.537	A(1,5,6)	107.19	A(7,19,22)	112.00	D(4,1,5,6)	57.695	D(19,7,9,12)	170.618
	R(7,8)	1.101	A(1,5,7)	113.85	A(20,19,21)	107.31	D(4,1,5,7)	174.290	D(5,7,19,20)	172.904
	R(7,9)	1.549	A(1,5,15)	110.49	A(20,19,22)	107.45	D(4,1,5,15)	-58.713	D(5,7,19,21)	-67.737
	R(7,19)	1.536	A(6,5,7)	105.76	A(21,19,22)	107.70	D(1,5,7,8)	173.994	D(5,7,19,22)	53.089
	R(9,10)	1.106	A(6,5,15)	107.13			D(1,5,7,9)	-70.144	D(8,7,19,20)	55.675
	R(9,11)	1.098	A(7,5,15)	111.97			D(1,5,7,19)	56.056	D(8,7,19,21)	175.034
	R(9,12)	1.491	A(5,7,8)	106.16			D(6,5,7,8)	-68.583	D(8,7,19,22)	-64.140
	R(12,13)	1.086	A(5,7,9)	112.29			D(6,5,7,9)	47.280	D(9,7,19,20)	-59.828
	R(12,14)	1.085	A(5,7,19)	113.89			D(6,5,7,19)	173.479	D(9,7,19,21)	59.531
	R(15,16)	1.096	A(8,7,9)	106.39			D(15,5,7,8)	47.769	D(9,7,19,22)	-179.643
	R(15,17)	1.096	A(8,7,19)	107.38			D(15,5,7,9)	163.631	D(7,9,12,13)	-40.313
	R(15,18)	1.096	A(9,7,19)	110.24			D(15,5,7,19)	-70.169	D(7,9,12,14)	150.162
	R(19,20)	1.095	A(7,9,10)	107.30			D(1,5,15,16)	178.015	D(10,9,12,13)	80.347
	R(19,21)	1.096	A(7,9,11)	110.05			D(1,5,15,17)	-61.376	D(10,9,12,14)	-89.178
	R(19,22)	1.094	A(7,9,12)	114.66			D(1,5,15,18)	58.153	D(11,9,12,13)	-165.012
			A(10,9,11)	104.74			D(6,5,15,16)	61.569	D(11,9,12,14)	25.463
			A(10,9,12)	109.52			D(6,5,15,17)	-177.822		
			A(11,9,12)	110.07			D(6,5,15,18)	-58.293		
			A(9,12,13)	120.35			D(7,5,15,16)	-53.952		
			A(9,12,14)	121.44			D(7,5,15,17)	66.657		
			A(13,12,14)	117.41			D(7,5,15,18)	-173.814		
			A(5,15,16)	111.39			D(5,7,9,10)	176.896		
			A(5,15,17)	111.91			D(5,7,9,11)	63.477		

Table S20: Vibrational Frequencies (cm^{-1}) for Optimized Alkane Isomer Species at the B3LYP/6-31G(d,p) Level of Theory.

Species	Frequencies									
***n*-c_7h_{16}**	68.14	83.53	98.40	146.64	151.31	243.76	245.41	247.63	301.48	416.28
	481.10	737.04	742.83	778.31	852.33	884.77	920.90	944.90	999.98	1033.16
	1041.81	1068.75	1069.56	1093.08	1160.78	1213.32	1249.34	1264.74	1300.83	1325.96
	1332.49	1340.68	1346.51	1378.59	1411.28	1416.81	1427.13	1428.34	1499.42	1500.28
	1503.69	1509.63	1513.51	1513.58	1517.86	1525.00	1530.07	3008.87	3009.20	3015.60
	3023.77	3027.50	3031.50	3036.82	3037.04	3037.27	3049.02	3062.04	3072.90	3104.94
	3105.29	3109.89	3110.03							
cjccccc	66.74	81.64	100.66	117.21	145.32	157.10	246.64	247.91	305.07	411.49
	461.75	490.87	732.38	740.81	784.38	862.79	894.17	921.20	993.18	1008.81
	1053.60	1059.14	1072.09	1089.33	1118.98	1164.86	1225.25	1259.37	1278.54	1316.74
	1324.35	1337.68	1342.52	1374.60	1406.67	1415.76	1427.29	1477.00	1482.89	1500.18
	1500.93	1509.12	1513.67	1519.75	1528.23	2927.85	3009.28	3012.36	3019.63	3024.51
	3028.72	3033.29	3037.26	3044.50	3061.75	3074.61	3105.38	3110.33	3153.65	3256.26
ccjccccc	45.17	69.81	96.58	110.62	123.13	151.09	249.02	252.17	306.03	401.82
	425.38	481.94	733.28	753.73	837.59	888.67	925.88	956.74	994.56	1006.12
	1049.68	1067.67	1081.28	1115.42	1142.48	1172.87	1230.58	1259.22	1291.34	1319.83
	1331.09	1337.17	1376.57	1410.89	1418.35	1426.67	1430.36	1481.06	1489.72	1499.12
	1500.20	1503.56	1514.29	1516.10	1526.30	2917.49	2955.34	3001.18	3009.38	3018.69
	3026.55	3035.07	3037.05	3043.04	3054.26	3071.38	3101.81	3105.28	3110.36	3163.39
cccjcccc	35.60	45.40	90.18	125.86	128.95	236.96	248.31	252.15	308.50	411.71
	416.83	482.59	733.20	766.96	793.11	888.31	918.67	934.08	1003.68	1040.11
	1046.88	1067.53	1083.23	1113.36	1142.89	1170.69	1238.33	1256.04	1276.99	1309.89
	1318.78	1333.87	1373.90	1409.50	1422.98	1428.09	1434.81	1477.61	1488.73	1501.00
	1511.44	1511.63	1514.52	1519.18	1525.09	2916.92	2927.98	3002.70	3014.91	3016.59
	3024.93	3037.69	3042.13	3043.95	3067.80	3105.84	3110.45	3110.75	3117.32	3146.60
ccccjccc	37.67	38.93	85.65	118.31	154.78	244.75	246.00	246.91	302.75	420.00
	424.37	482.25	733.09	746.47	851.14	874.96	885.35	918.26	1003.44	1048.55
	1055.16	1068.35	1091.40	1111.49	1142.48	1170.43	1248.17	1257.70	1261.51	1320.45
	1324.02	1328.88	1375.01	1406.66	1425.22	1426.09	1437.24	1476.96	1487.68	1505.58
	1505.97	1513.48	1513.50	1522.18	1522.63	2914.36	2919.45	3003.60	3008.52	3029.46
	3029.97	3036.78	3037.06	3064.72	3065.12	3104.99	3105.18	3111.15	3111.28	3145.90
cc2cccc	58.60	81.26	127.78	144.14	224.32	246.02	254.57	300.25	303.09	406.85
	435.50	478.73	738.56	790.54	826.36	906.53	918.61	932.14	953.04	970.11
	1031.55	1046.75	1069.88	1093.20	1169.19	1196.82	1208.65	1258.51	1284.39	1323.84
	1338.25	1347.66	1377.17	1391.22	1412.81	1417.23	1427.14	1435.54	1492.65	1500.70
	1503.05	1508.55	1513.54	1514.38	1519.57	1524.42	1526.62	3000.41	3006.37	3015.07
	3024.86	3029.73	3035.58	3036.52	3038.71	3048.44	3071.97	3095.65	3101.78	3105.05
	3106.76	3110.10	3116.48							

cjc2cccc	69.27	80.71	123.76	133.51	153.87	243.22	247.48	287.54	297.66	380.88
	428.65	469.87	547.23	739.53	794.09	843.14	906.95	911.01	937.02	964.93
	1018.32	1038.40	1047.55	1072.65	1117.43	1171.25	1201.48	1254.22	1280.26	1318.72
	1325.55	1337.26	1367.41	1387.34	1405.78	1416.04	1427.02	1475.55	1498.74	1501.40
	1508.06	1511.34	1513.64	1515.59	1526.07	2997.09	3009.12	3014.94	3024.44	3033.43
	3036.81	3039.25	3049.10	3070.35	3104.39	3105.09	3110.10	3116.28	3144.88	3248.30
ccj2cccc	35.39	81.32	97.88	114.11	127.20	130.50	237.57	252.21	320.22	391.13
	410.92	462.27	737.49	774.90	794.84	901.12	931.04	947.93	977.40	987.83
	1014.24	1050.41	1056.05	1082.84	1120.32	1231.87	1269.25	1290.48	1304.74	1333.76
	1349.56	1357.33	1395.63	1411.83	1427.14	1429.38	1482.31	1485.84	1492.64	1497.97
	1499.59	1510.09	1511.79	1515.29	1524.00	2948.50	2954.46	2998.55	3017.44	3025.90
	3034.94	3036.99	3040.99	3043.26	3046.63	3071.58	3092.71	3094.93	3105.27	3109.18
cc2cjccc	32.71	49.36	103.71	164.86	232.75	244.08	258.03	277.23	298.69	356.04
	415.84	477.40	534.14	741.55	829.82	867.63	901.72	929.28	943.34	963.21
	1045.37	1063.55	1087.99	1105.58	1131.73	1183.34	1195.78	1254.50	1271.77	1323.20
	1333.60	1342.65	1391.44	1407.36	1422.98	1425.94	1438.08	1482.45	1501.74	1503.94
	1505.50	1513.16	1516.17	1522.42	1524.22	2918.08	2994.68	3011.62	3030.45	3031.69
	3036.28	3036.92	3065.66	3099.47	3104.93	3105.22	3111.12	3113.90	3115.64	3137.46
cc2ccjcc	42.53	46.54	104.93	170.28	228.25	245.74	254.11	291.99	308.57	404.64
	425.89	453.81	482.40	770.40	816.09	867.71	914.83	934.65	952.23	969.68
	1033.94	1049.70	1082.26	1121.42	1142.92	1184.33	1197.02	1245.81	1273.60	1278.82
	1343.17	1370.40	1387.54	1413.94	1424.15	1428.72	1436.90	1474.85	1486.97	1501.56
	1507.71	1512.07	1517.09	1519.63	1523.08	2919.65	2927.38	2999.63	3013.94	3018.43
	3029.90	3035.08	3042.25	3096.23	3101.84	3107.39	3110.53	3115.44	3117.33	3140.86
cc2cccjc	48.08	75.23	104.31	114.08	149.60	225.48	250.11	298.82	307.69	402.31
	416.13	441.94	477.27	754.97	823.55	910.18	930.78	933.32	958.33	971.30
	997.27	1046.13	1082.94	1122.55	1143.26	1177.21	1197.41	1232.45	1278.17	1314.10
	1343.95	1376.47	1389.61	1415.05	1418.61	1429.35	1435.17	1480.09	1489.66	1497.70
	1501.24	1503.67	1510.93	1519.82	1524.82	2912.43	2955.30	3001.46	3014.93	3023.23
	3030.50	3036.43	3042.46	3057.11	3096.41	3101.80	3102.44	3107.05	3115.15	3162.19
cc2ccccj	61.49	82.43	117.43	130.65	150.85	223.93	252.79	301.64	306.21	407.37
	434.63	455.46	491.82	732.54	805.20	831.34	897.73	931.96	948.98	968.29
	1003.64	1050.22	1063.23	1088.30	1125.34	1174.12	1196.75	1220.48	1275.12	1302.93
	1333.67	1343.76	1375.85	1389.14	1410.42	1416.82	1435.87	1475.94	1482.04	1492.89
	1502.99	1508.88	1515.72	1519.61	1525.77	2926.81	3000.72	3007.18	3019.12	3029.58
	3030.70	3036.17	3041.82	3079.35	3096.26	3102.24	3107.09	3117.21	3153.46	3256.15
cc2c2cc	58.13	86.93	204.47	211.92	232.04	248.83	260.95	297.41	321.45	339.01
	432.53	461.95	560.27	753.02	791.32	857.65	925.93	934.12	969.29	976.95
	983.85	1039.79	1054.30	1079.50	1148.94	1187.61	1198.43	1216.99	1300.67	1318.33
	1344.20	1370.15	1392.93	1395.57	1417.50	1427.07	1430.90	1438.96	1498.56	1502.92
	1506.24	1512.18	1519.10	1521.70	1524.52	1526.39	1530.56	2990.73	3005.40	3022.43
	3035.74	3039.56	3042.01	3048.84	3058.37	3101.77	3105.11	3106.64	3107.90	3112.05
	3116.51	3118.26	3122.93							

cjc2c2cc	78.39	85.23	132.69	206.80	213.14	233.91	244.35	280.36	312.84	345.13
	424.12	449.62	503.30	592.65	746.44	793.44	863.38	910.86	956.90	975.06
	995.01	1018.58	1038.46	1065.10	1119.17	1155.57	1190.33	1213.52	1285.34	1301.08
	1310.86	1355.01	1375.52	1398.55	1418.80	1424.78	1429.19	1474.81	1497.92	1507.73
	1512.74	1515.50	1519.29	1523.84	1525.56	2906.11	2996.24	3026.95	3038.61	3040.90
	3048.29	3063.08	3103.94	3105.95	3111.25	3114.10	3118.97	3125.42	3147.25	3249.87
ccj2c2cc	36.93	95.18	112.34	127.74	175.16	220.08	222.41	243.70	287.10	357.45
	404.50	464.92	510.22	696.56	806.36	849.27	945.42	948.87	979.72	985.32
	1004.96	1020.18	1049.52	1094.21	1102.13	1170.82	1241.58	1286.83	1306.90	1329.49
	1377.40	1396.15	1412.39	1412.79	1424.35	1431.41	1483.47	1487.97	1495.10	1501.33
	1508.76	1511.25	1512.84	1515.12	1522.49	2944.05	2957.50	3008.89	3026.35	3035.12
	3038.71	3043.84	3046.44	3059.28	3095.55	3102.99	3105.02	3106.90	3111.82	3114.95
cc2cj2cc	42.33	44.54	104.17	147.21	214.87	231.72	248.48	265.01	294.82	334.15
	413.77	477.07	528.58	697.30	788.58	862.56	927.81	928.88	955.06	985.72
	993.11	1035.35	1056.61	1094.19	1097.43	1178.07	1240.74	1257.89	1341.33	1345.77
	1348.93	1388.87	1405.08	1415.21	1419.48	1431.20	1484.98	1494.53	1498.56	1500.59
	1509.56	1511.54	1518.21	1519.65	1524.28	2960.64	3006.33	3019.92	3033.57	3036.83
	3038.17	3044.32	3047.75	3095.26	3100.71	3106.59	3107.31	3112.64	3115.15	3116.65
cc2c2jcc	80.48	106.73	153.98	194.94	229.70	235.90	251.83	276.79	311.81	340.25
	432.34	445.88	474.91	606.95	773.89	795.01	856.60	933.25	948.42	967.64
	974.41	996.69	1048.83	1080.94	1102.10	1180.53	1189.59	1201.49	1284.57	1297.66
	1319.75	1370.06	1384.11	1393.81	1415.25	1425.99	1433.33	1479.43	1503.49	1503.84
	1509.24	1512.08	1520.27	1521.99	1526.36	2979.44	3008.27	3027.26	3034.97	3039.01
	3041.72	3063.26	3103.89	3105.25	3107.19	3110.12	3114.86	3117.24	3152.65	3254.84
cc2c2cjc	54.49	78.71	118.77	201.75	220.21	222.87	259.97	275.95	338.78	367.23
	413.70	450.00	467.66	538.66	789.05	863.81	930.16	933.77	963.08	971.85
	993.75	1015.22	1045.49	1094.05	1140.02	1184.70	1192.54	1202.45	1281.96	1320.35
	1355.80	1373.43	1404.74	1412.32	1419.24	1425.08	1433.91	1488.84	1499.59	1501.68
	1503.52	1510.98	1513.47	1521.09	1531.66	2954.62	2980.32	2999.87	3032.23	3037.22
	3039.79	3046.63	3096.08	3099.06	3102.49	3109.84	3113.92	3119.14	3125.21	3148.05
cc2c2ccj	57.19	129.07	131.64	205.33	220.14	241.42	263.62	275.93	289.04	380.88
	423.91	459.74	496.42	555.25	724.85	821.77	887.26	928.85	936.62	968.76
	970.61	1012.98	1046.12	1084.01	1126.82	1167.31	1186.43	1207.29	1235.78	1313.83
	1347.00	1355.48	1390.83	1395.53	1417.08	1424.83	1438.48	1474.14	1483.10	1501.42
	1506.01	1513.81	1522.47	1525.51	1527.45	2932.36	2997.37	3016.11	3034.56	3040.82
	3043.62	3047.96	3100.92	3104.33	3105.90	3110.01	3114.60	3119.33	3151.55	3254.28

Table S21: Moments of Inertia[a] for Optimized Alkane Isomer Species at the B3LYP/6-31G(d,p) Level of Theory.

Species	I_a	I_b	I_c
***n*-c_7h_{16}**	149.58338	2509.17715	2580.87717
cjccccc	142.72611	2440.64744	2514.26322
ccjccccc	137.80568	2490.14161	2555.29526
cccjcccc	159.65346	2456.92481	2535.13885
ccccjccc	146.35318	2489.69086	2546.02118
cc2cccc	296.78839	1825.56851	2006.56789
cjc2cccc	282.39955	1800.63004	1963.78143
ccj2cccc	339.80474	1752.19184	1862.59800
cc2cjccc	292.60868	1846.28346	2020.68490
cc2ccjcc	301.45487	1744.00999	1921.52743
cc2cccjc	286.73865	1801.90682	1989.36238
cc2ccccj	290.62937	1771.43227	1947.67958
cc2c2cc	458.24033	1223.93298	1315.69979
cjc2c2cc	529.28271	1056.92220	1245.89127
ccj2c2cc	650.56073	955.76187	1147.90634
cc2cj2cc	539.15082	1117.88842	1192.40082
cc2c2jcc	439.31414	1198.33515	1301.90982
cc2c2cjc	498.62236	1053.43236	1424.50165
cc2c2ccj	588.22509	995.55667	1145.85526

[a]Units in AMU $Bohr^2$

Table S22: Comparison of Different Selected Torsion Frequencies to Represent the Vibrations Replaced by the Pitzer-Gwinn and ROTATOR analysis of the Internal Rotor Contributions.[a]

Species	$S^{\circ}(T)$ (cal mol^{-1} K^{-1}) from TVR Contributions							Frequencies Included (cm^{-1})							
	298 K	400 K	500 K	600 K	800 K	1000 K	1500 K								
***n*-c_7h_{16}**								**68.14**	**83.53**	**98.40**	**146.64**	**151.31**	**243.76**	**245.41**	**247.63**
	71.068	79.811	88.858	98.040	115.959	132.722	168.989	•	•	•	•	•	•		
	73.510	82.299	91.366	100.560	118.490	135.258	171.531		•	•	•	•	•	•	
	73.526	82.315	91.383	100.578	118.508	135.276	171.549		•	•	•	•	•		•
	72.790	81.574	90.639	99.832	117.762	134.529	170.801	•	•		•	•	•	•	
	72.806	81.591	90.657	99.850	117.779	134.547	170.819	•	•		•	•	•		•
	71.080	79.823	88.871	98.053	115.972	132.735	169.002	•	•	•	•	•		•	
	71.096	79.840	88.888	98.071	115.990	132.753	169.020	•	•	•	•	•			•
	72.818	81.603	90.669	99.863	117.792	134.560	170.832	•	•		•	•		•	•
cc2cccc								**58.60**	**81.26**	**127.78**	**144.14**	**224.32**	**246.02**	**254.57**	
	70.650	79.603	88.786	98.057	116.075	132.884	169.191	•	•	•	•	•	•		
	72.811	81.811	91.015	100.299	118.329	135.143	171.456	•		•	•	•	•	•	
	71.930	80.922	90.123	99.404	117.432	134.245	170.557	•	•		•	•	•	•	
cc2c2cc								**58.13**	**86.93**	**204.47**	**211.92**	**232.04**	**248.83**	**260.95**	
	70.038	79.198	88.506	97.855	115.949	132.787	169.104	•	•	•	•	•	•		
	72.110	81.319	90.650	100.011	118.117	134.961	171.284	•		•	•	•	•	•	
	70.474	79.655	88.973	98.327	116.427	133.267	169.587	•	•		•	•	•	•	

[a]Contributions from only Translations, Rotations, and Vibrations using the SMCPS code are shown.