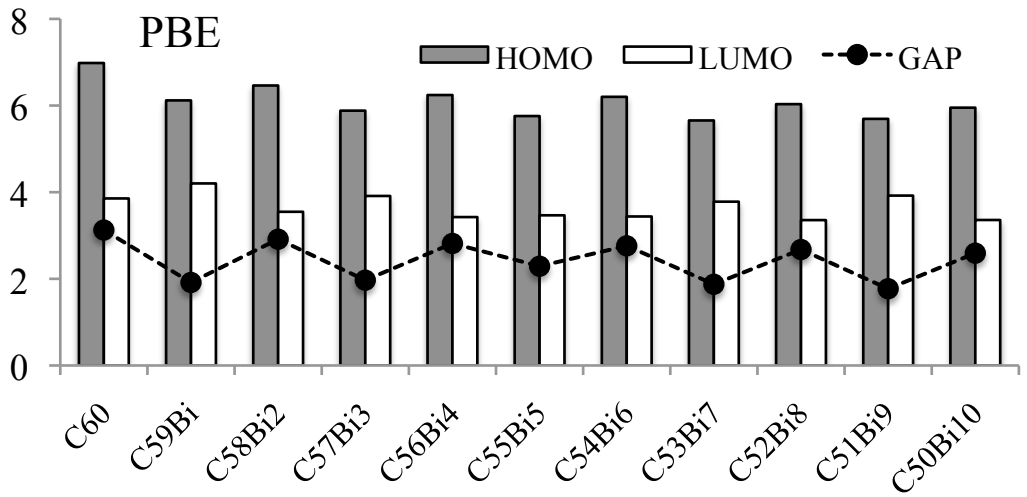
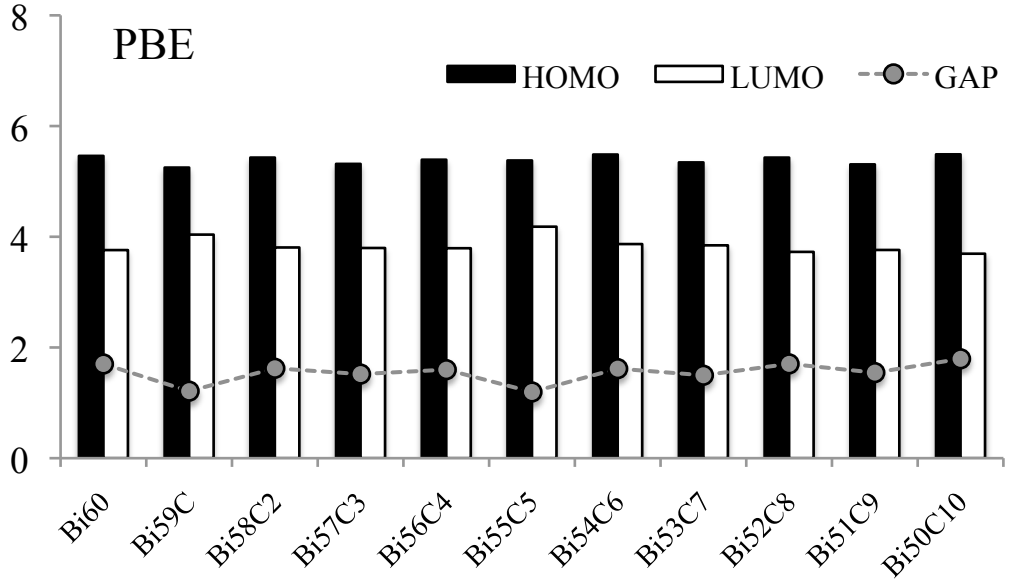
Reactivity Indexes of Fullerene and Bismullene Mixed Clusters: How the *Intruders* Modify the Properties?

Ana Martínez[1]
Departamento de Materiales de Baja Dimensionalidad, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Circuito Exterior s/n, Ciudad Universitaria, P.O. Box 70-360, Coyoacán, 04510, Ciudad de México, México

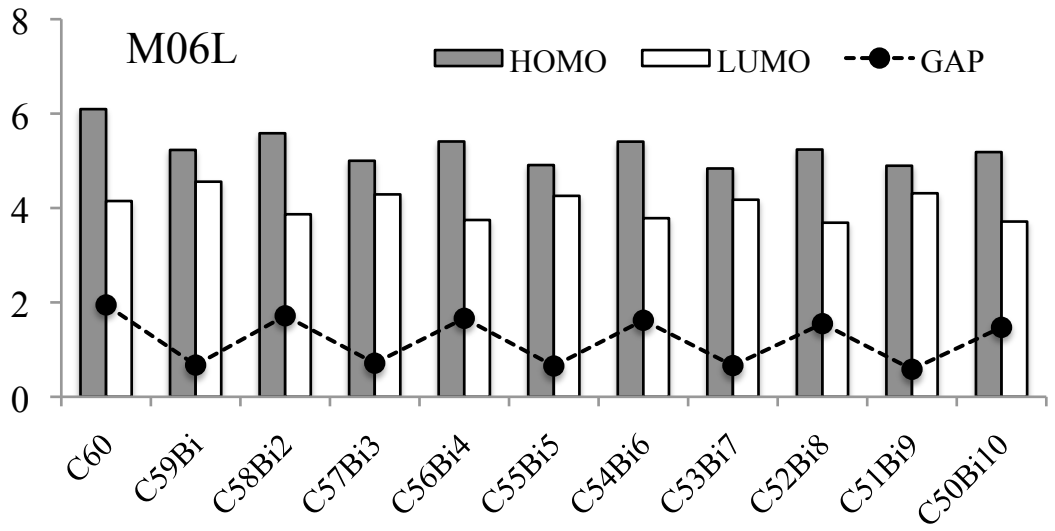
SUPORTING INFORMATION

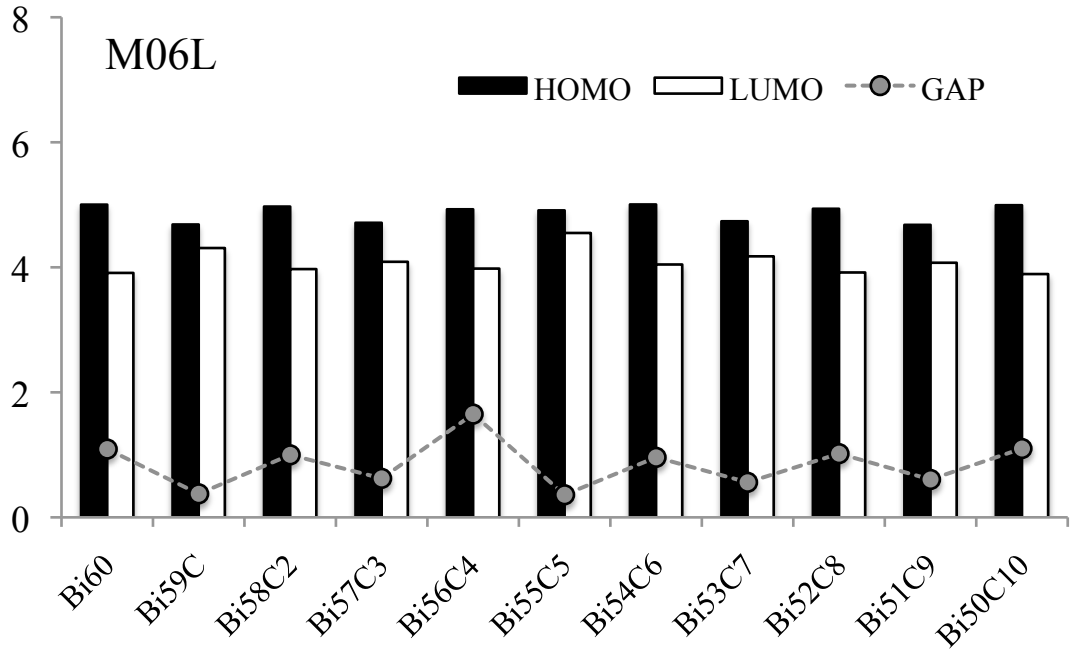
HOMO, LUMO and HOMO-LUMO gaps of the most stable structures are reported. These values were obtained with two different functionals: PBE and M06L.





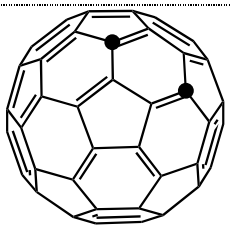
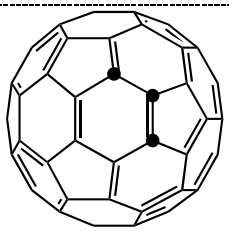
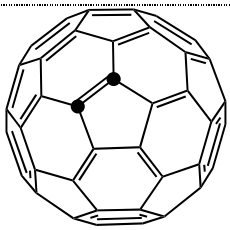
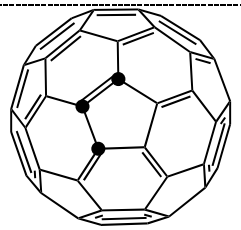
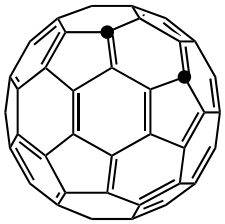
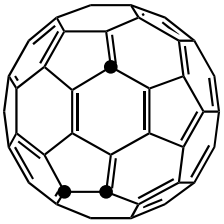
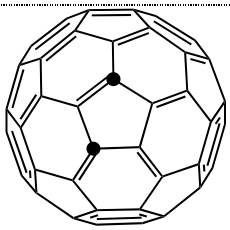
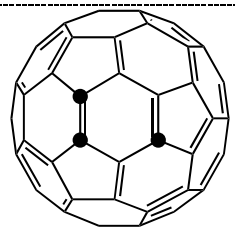
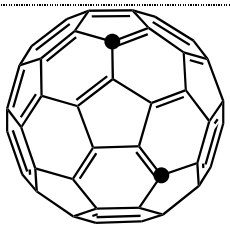
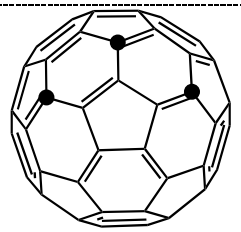
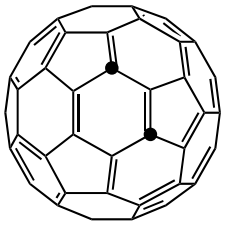
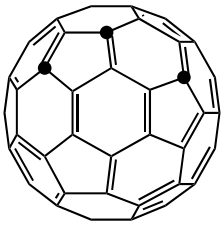
[1] Corresponding author: martina@unam.mx

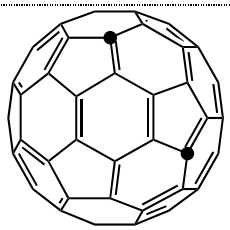
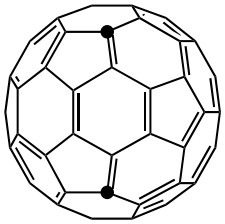
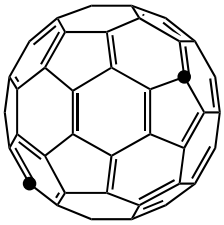

M06L
HOMO
LUMO
GAP
8
6
4
2
0
C60
C59Bi
C58Bi2
C57Bi3
C56Bi4
C55Bi5
C54Bi6
C53Bi7
C52Bi8
C51Bi9
C50Bi10

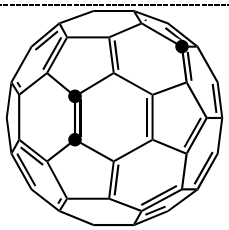
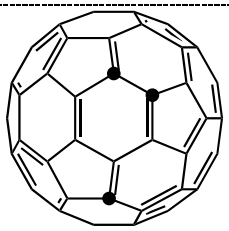
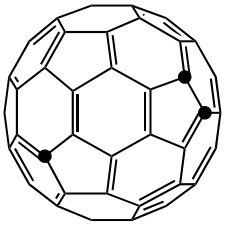
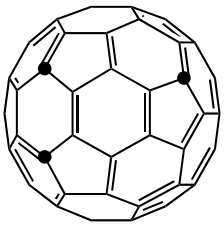
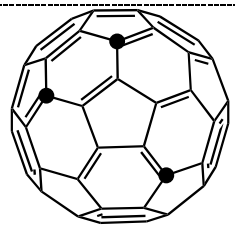
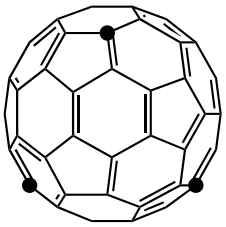
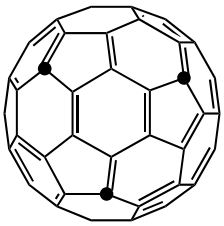

M06L
HOMO
LUMO
GAP
8
6
4
2
0
Bi60
Bi59C
Bi58C2
Bi57C3
Bi56C4
Bi55C5
Bi54C6
Bi53C7
Bi52C8
Bi51C9
Bi50C10

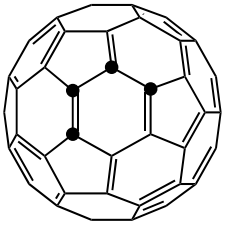
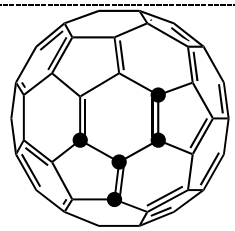
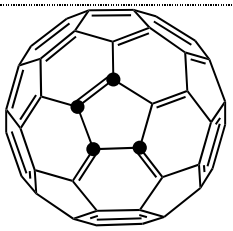
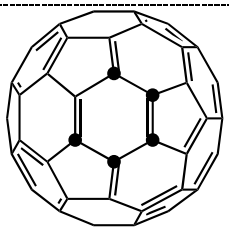
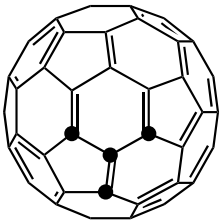
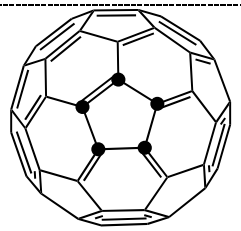
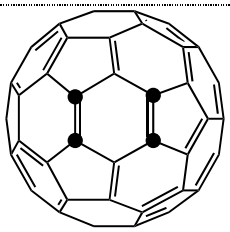
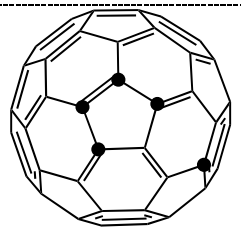
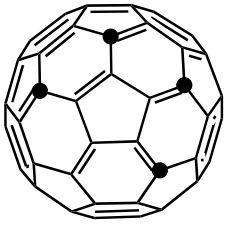
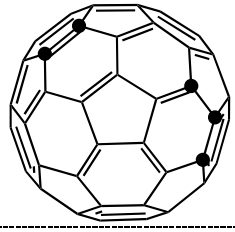
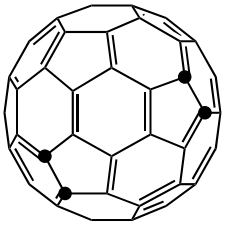
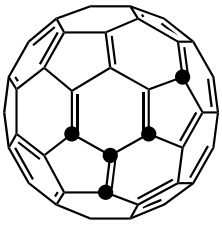
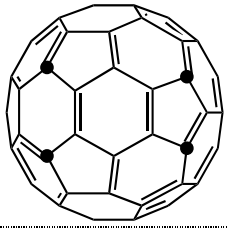
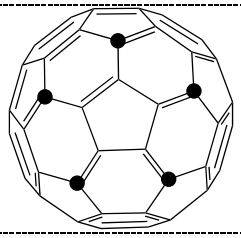
Schematic representation of the initial structures that were optimized and total energies of the optimized geometries are reported.

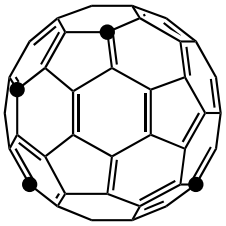
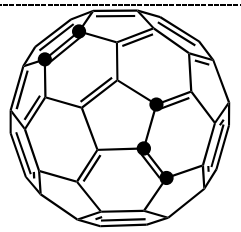
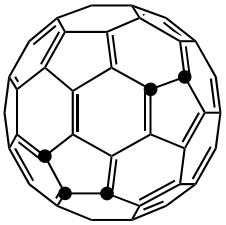
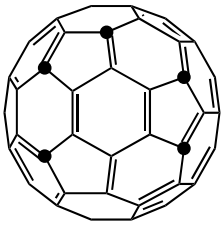
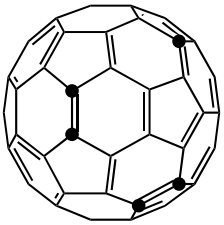
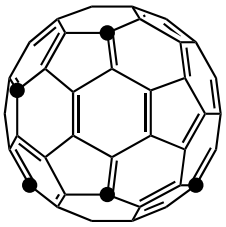
Fullerene like systems

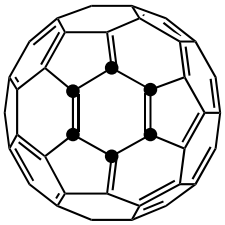
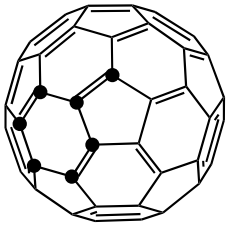
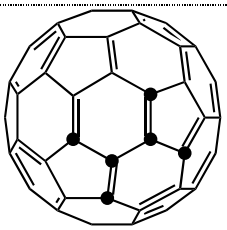
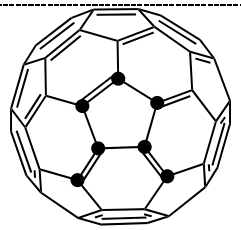
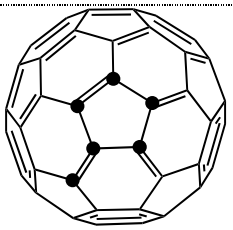
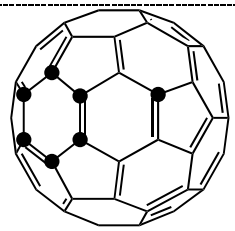
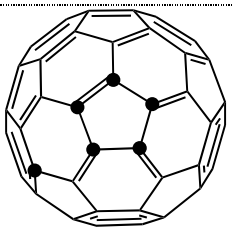
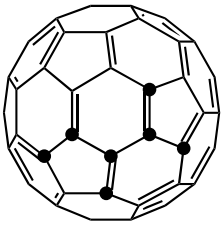
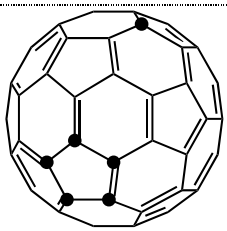
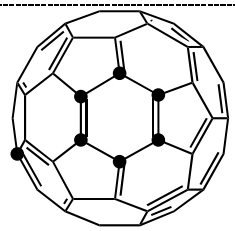
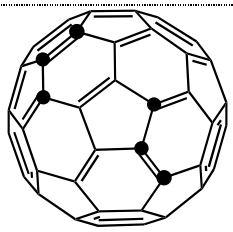
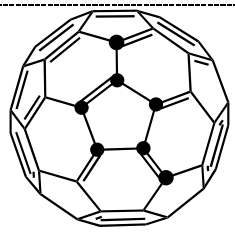
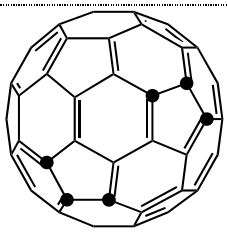
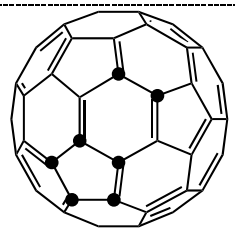
$C_{58}Bi_2$		$C_{57}Bi_3$	
Initial Structure	Total Energy (au)	Initial Structure	Total Energy (au)
	-2218.88546877		-2186.266896
	-2218.8779237		-2186.25730694
	-2218.82673596		-2186.24872622
	-2218.82673596		-2186.24557402
	-2218.81107315		-2186.23180656
	-2218.80710379		-2186.21101278

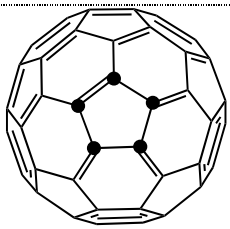
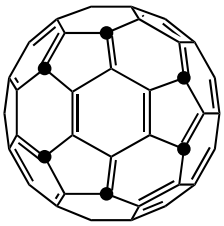
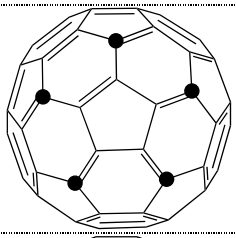
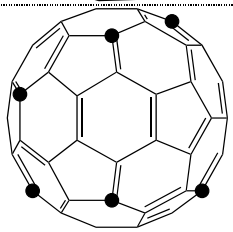
	-2218.80455239
	-2218.80230488
	-2218.778795 random distribution no Bi-Bi bond

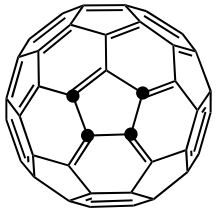
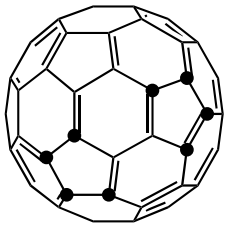
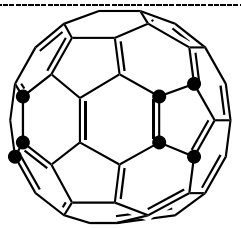
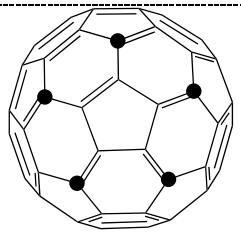
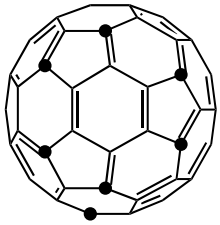
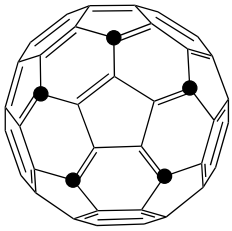
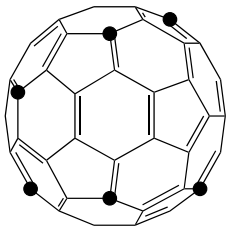
	-2186.19192550
	-2186.19014978
	-2186.18934776
	-2186.18553752
	-2186.17909811
	-2186.139905 random distribution no Bi-Bi bond
	-2186.09950496

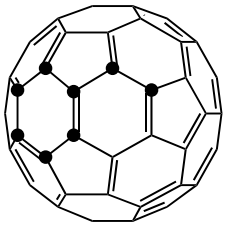
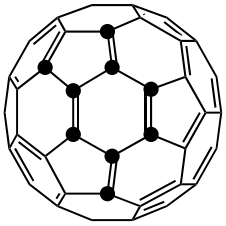
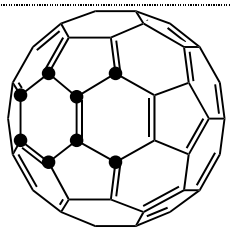
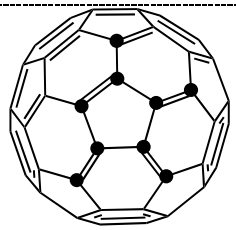
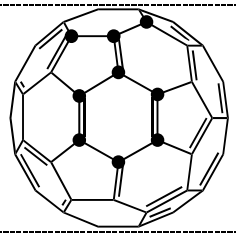
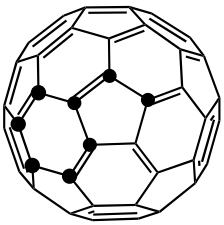
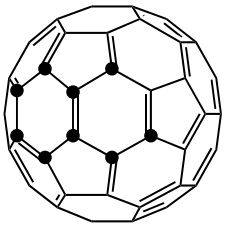
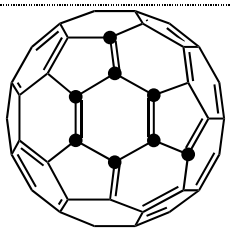
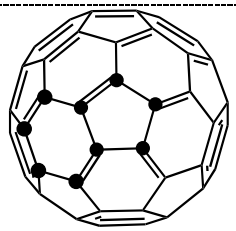
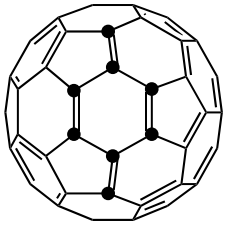
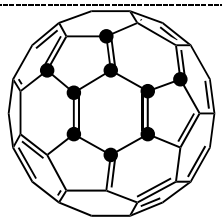
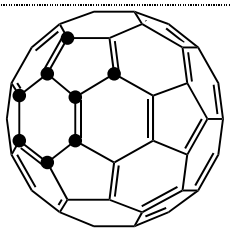
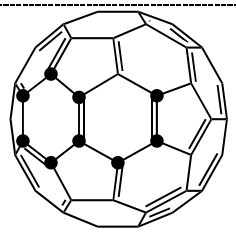
$C_{56}Bi_4$		$C_{55}Bi_5$	
Initial Structure	Total Energy (au)	Initial Structure	Total Energy (au)
	-2153.684899		-2121.04661837
	-2153.63953984		-2121.0423079
	-2153.61145849		-2121.0415660
	-2153.60483339		-2120.98080156
	-2153.59156937		-2120.96842710
	-2153.56559680		-2120.96668020
	-2153.50385776		-2120.96393361

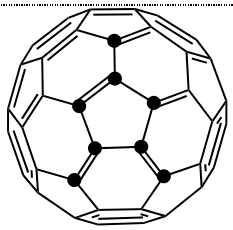
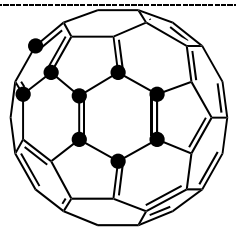
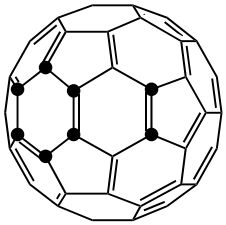
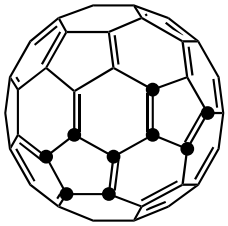
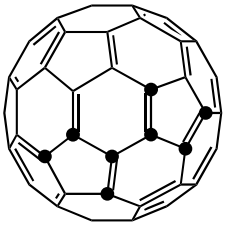
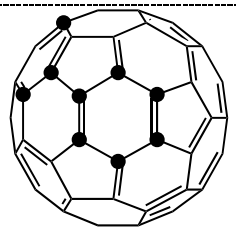
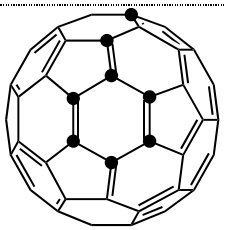
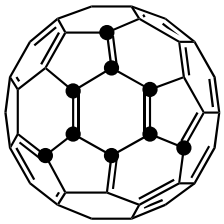
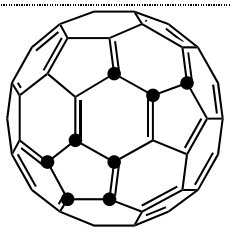
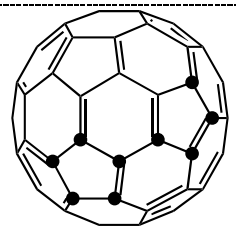
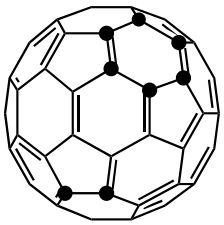
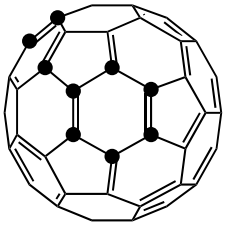
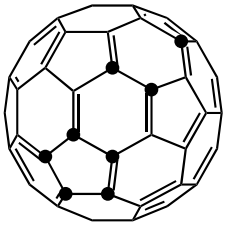
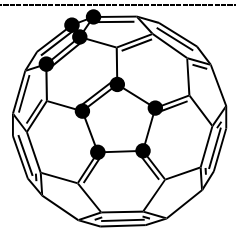
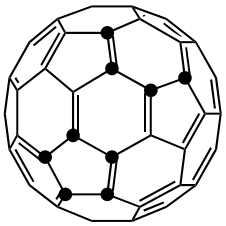
	-2153.4116459 random distribution no Bi-Bi bond		-2120.93722119
			-2120.91537932
			-2120.89682327
			-2120.86998144
			-2120.725006 random distribution no Bi-Bi bond

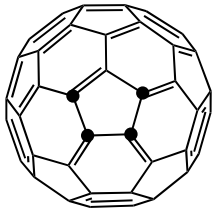
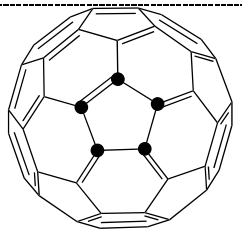
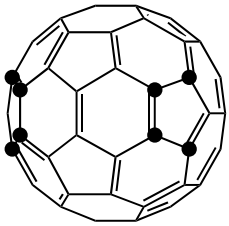
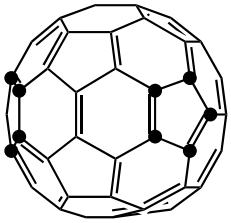
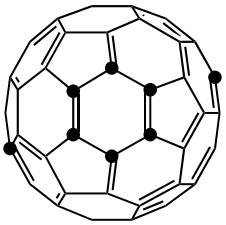
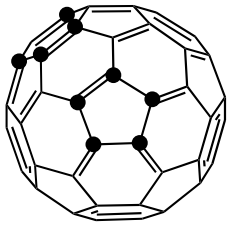
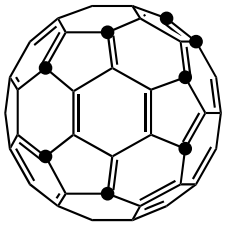
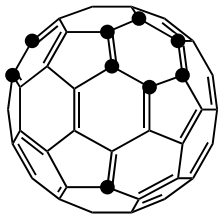
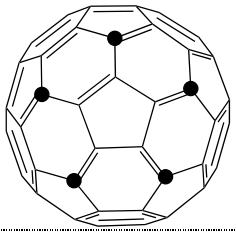
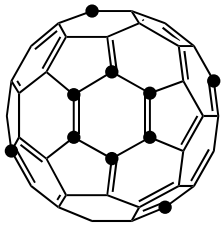
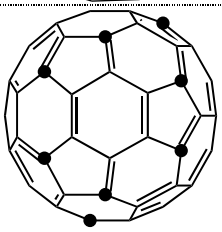
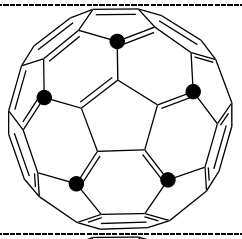
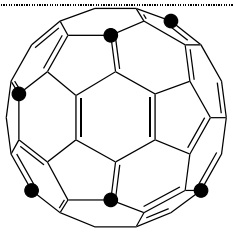
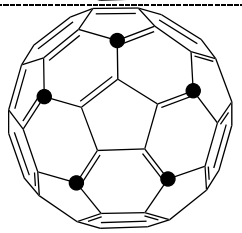
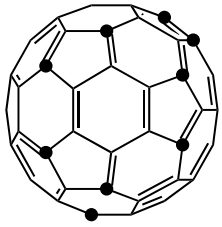
$C_{54}Bi_6$		$C_{53}Bi_7$	
Initial Structure	Total Energy (au)	Initial Structure	Total Energy (au)
	-2088.479889		-2055.851698
	-2088.45412041		-2055.82934332
	-2088.42987272		-2055.82335963
	-2088.40717729		-2055.82009970
	-2088.36284051		-2055.79544698
	-2088.32069113		-2055.78890330
	-2088.31762831		-2055.77688575

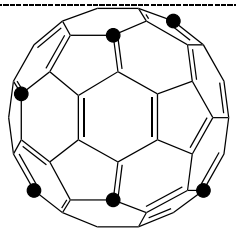
	-2088.28376962 one Bi atom at the opposite equivalent positions
	-2088.2837696
	-2088.25071956
	-2088.010608 random distribution no Bi-Bi bond

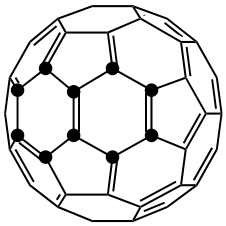
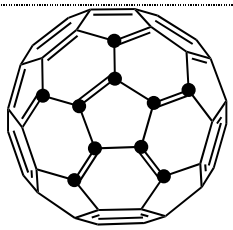
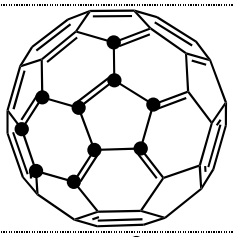
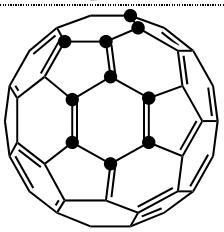
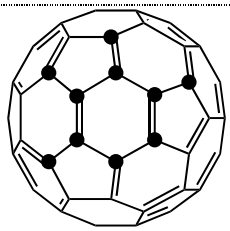
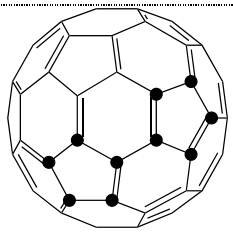
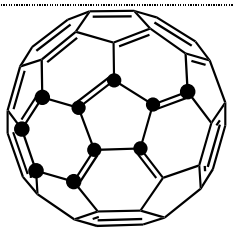
	-2055.71374211 other three Bi atoms at the opposite equivalent positions
	-2055.71358789
	-2055.70439229
	-2055.65054178 other two Bi atoms at the opposite equivalent positions
	-2055.59724455
	-2055.57406474 other two Bi atoms random positions no Bi-Bi bond
	-2055.376740 random distribution, no Bi-Bi bond

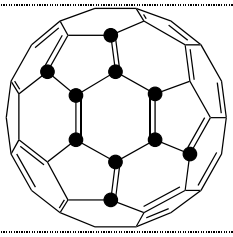
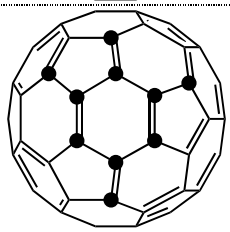
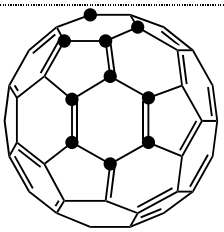
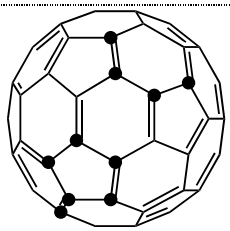
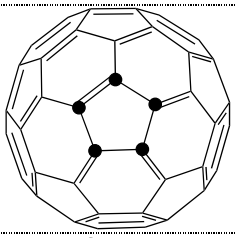
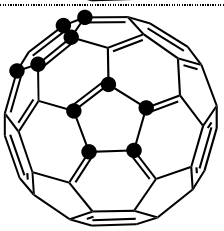
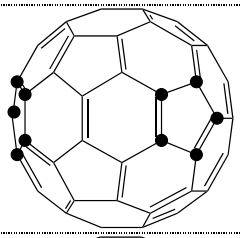
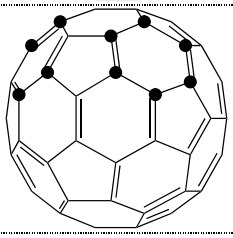
$C_{52}Bi_8$		$C_{51}Bi_9$	
Initial Structure	Total Energy (au)	Initial Structure	Total Energy (au)
	-2023.26917703		-1990.630748
	-2023.25961225		-1990.63011331
	-2023.22475442		-1990.62793434
	-2023.22431368		-1990.62786360
	-2023.22146050		-1990.62537642
	-2023.218657		-1990.62046349
	-2023.20286865		-1990.61990193

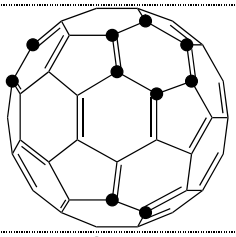
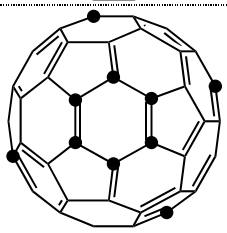
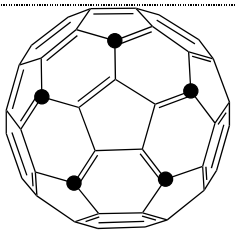
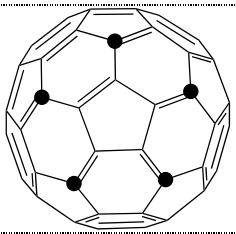
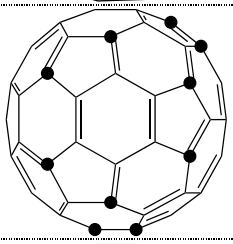
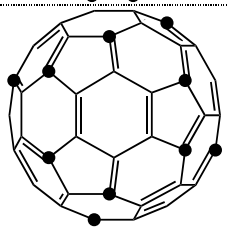
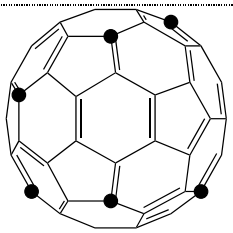
	-2023.18817877		-1990.61894434
	-2023.18677399		-1990.60284931
	-2023.17587375		-1990.60108713
	-2023.15782768		-1990.59513294
	-2023.13743189		-1990.57786503
	-2023.13415635		-1990.56353220
	-2023.12517329		-1990.55765901
	-2023.10031483		-1990.53164920

	-2023.09890593 other four Bi atoms at the opposite equivalent positions		-1990.49805535 other four Bi atoms at the opposite equivalent positions
	-2023.08007826		-1990.48470637
	-2023.07495103		-1990.47721859
	-2022.95596170		-1990.45561521
	-2022.92446966 other three Bi atoms at the opposite equivalent positions		-1990.41898431
	-2022.86603353		-1990.34741687 other four Bi atoms at the opposite equivalent positions
	-2022.659604 random distribution, no Bi-Bi bond		-1990.32815654 other four Bi atoms at the other equivalent positions, not symmetric, not the opposite
			-1990.25115415

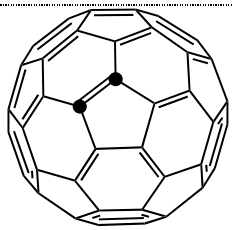
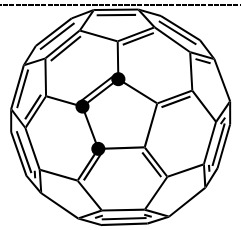
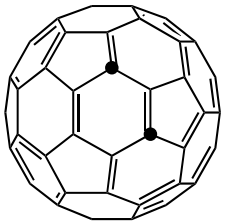
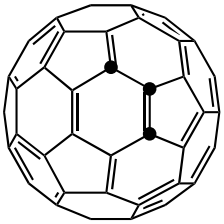
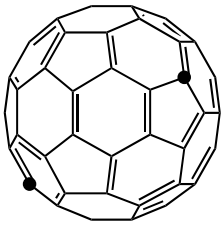
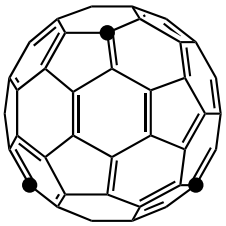
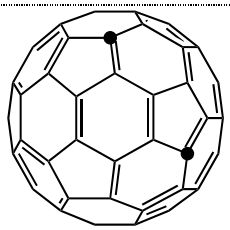
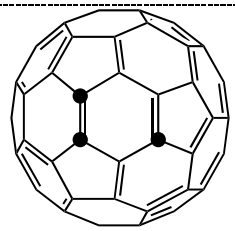
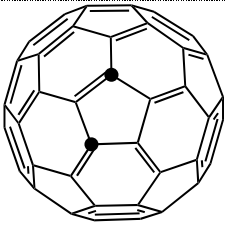
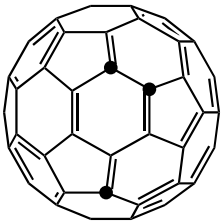
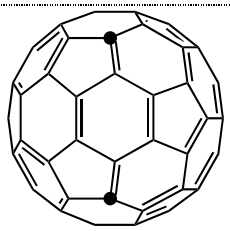
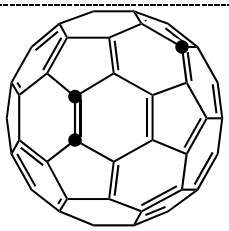
	-1990.026897 random distribution, no Bi-Bi bond

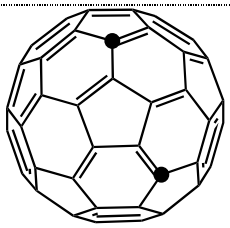
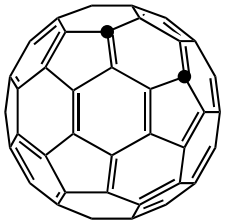
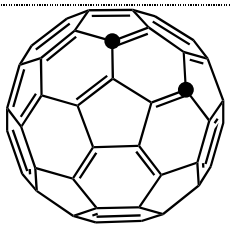
$C_{50}Bi_{10}$	
Initial Structure	Total Energy (au)
	-1958.06030874
	-1958.05741636
	-1958.03580626
	-1958.03132667
	-1958.02825580
	-1958.01713494
	-1957.98716284

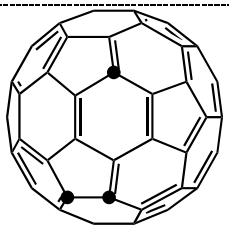
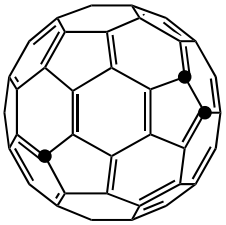
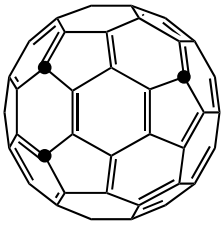
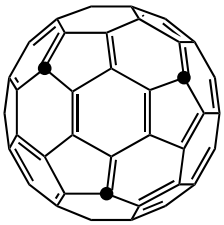
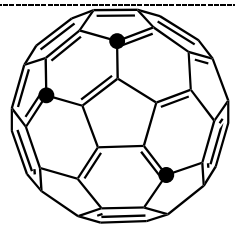
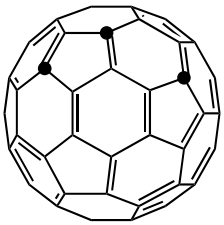
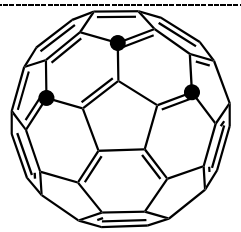
	-1957.9810411
	-1957.96576910
	-1957.94779493
	-1957.91866165
	-1957.89690501 other five Bi atoms at the opposite equivalent positions
	-1957.89671486
	-1957.8855084
	-1957.88348629

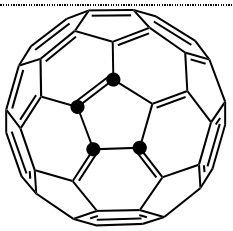
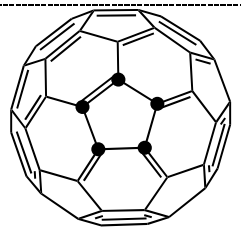
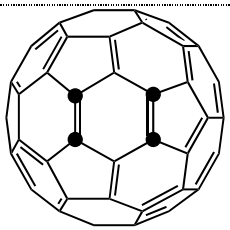
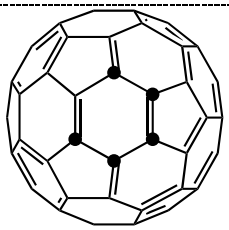
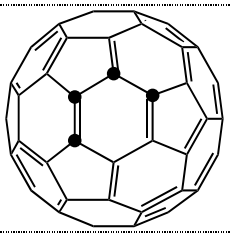
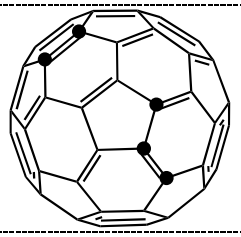
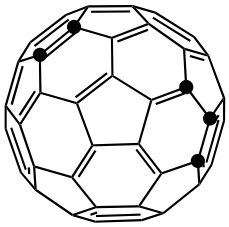
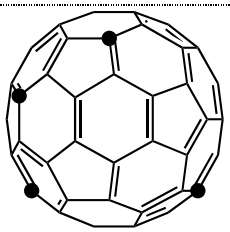
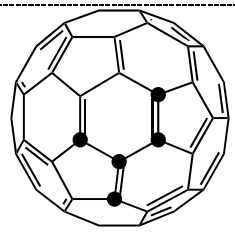
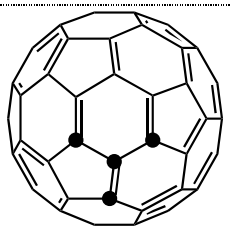
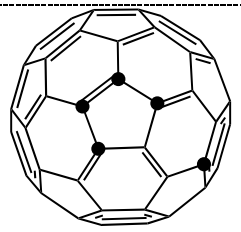
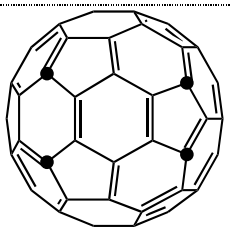
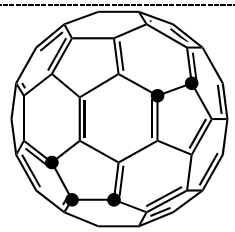
	-1957.84672542
	-1957.69165428
	-1957.67527241 other five Bi atoms at the other equivalent positions, not symmetric, not the opposite
	-1957.66876746 other five Bi atoms at the opposite equivalent positions
	-1957.62759059
	-1957.34049637 no Bi-Bi bond
	-1957.321497 random distribution, no Bi-Bi bond

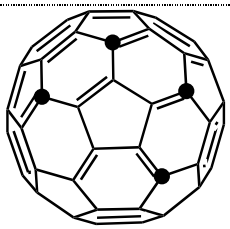
Bismullene like systems

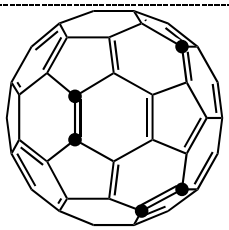
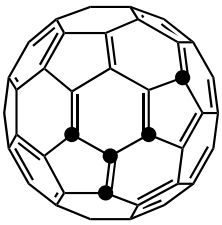
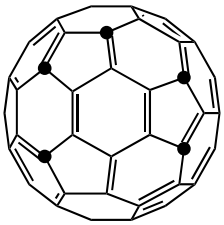
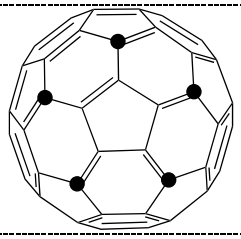
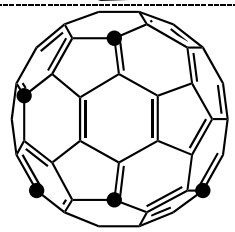
$Bi_{58}C_2$		$Bi_{57}C_3$	
Initial Structure	Total Energy (au)	Initial Structure	Total Energy (au)
	-393.156606		-425.709171
	-393.153860890		-425.707019430
	-393.147083 random distribution no C-C bond		-425.682260 random distribution no C-C bond
	-393.131716781		-425.682215988
	-393.12848678		-425.680315483
	-393.128005012		-425.676272370

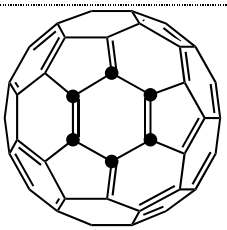
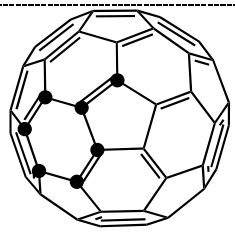
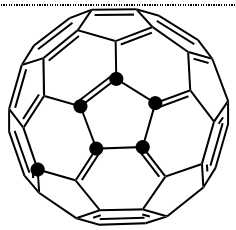
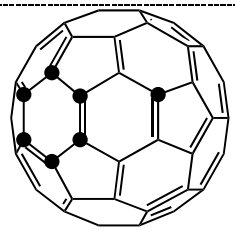
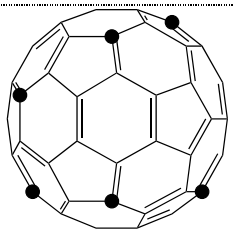
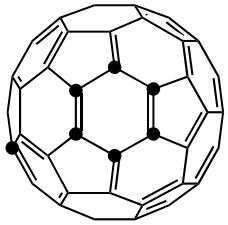
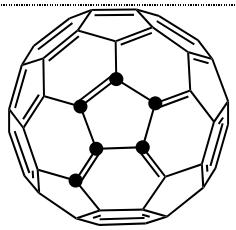
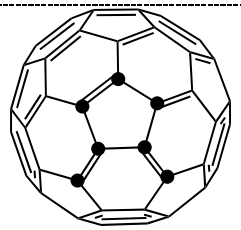
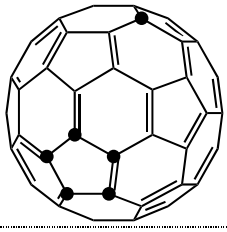
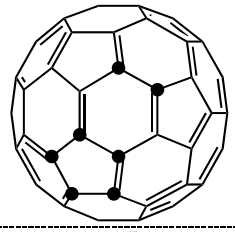
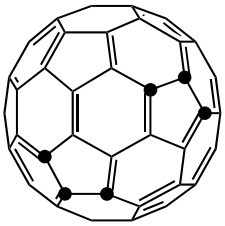
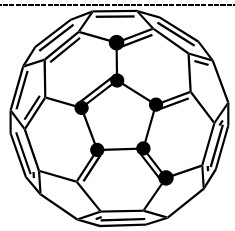
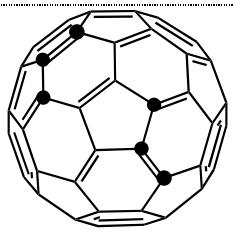
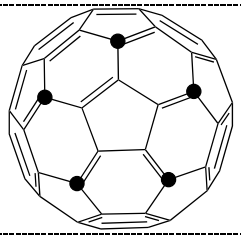
	-393.121128797
	-393.082542962
	-393.082545765

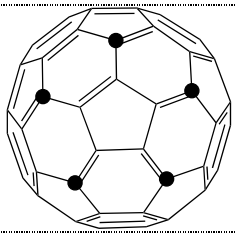
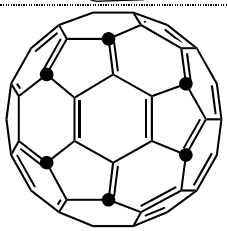
	-425.675866194
	-425.675644207
	-425.650423012
	-425.634738152
	-425.597647567
	-425.596104733
	-425.604595950

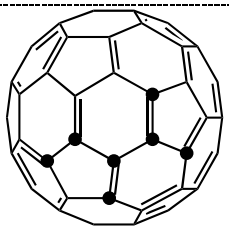
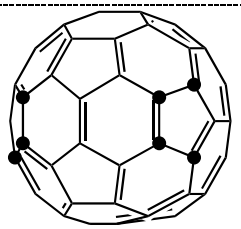
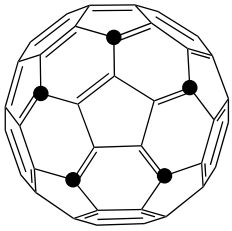
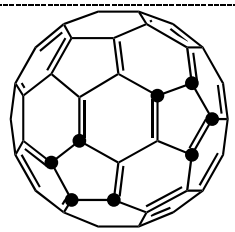
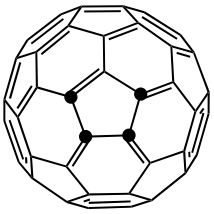
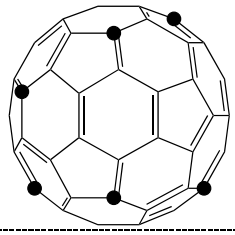
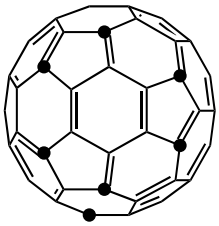
$Bi_{56}C_4$		$Bi_{55}C_5$	
Initial Structure	Total Energy (au)	Initial Structure	Total Energy (au)
	-458.308524		-490.914472562
	-458.3052125		-490.891851
	-458.303718101		-490.844124945
	-458.287016		-490.841139542
	-458.228987088 random distribution no C-C bond		-490.840988718
	-458.222411014		-490.840717419
	-458.178431722		-490.839494093

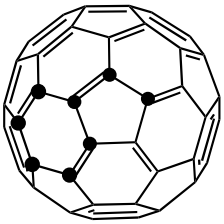
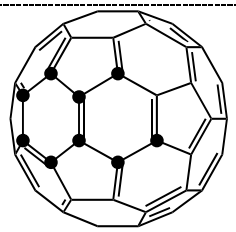
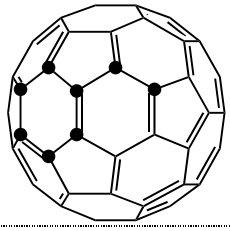
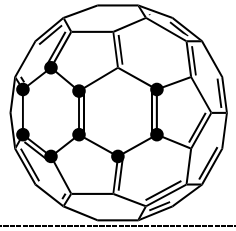
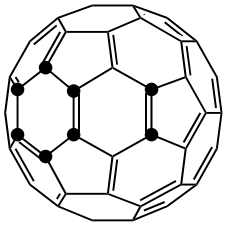
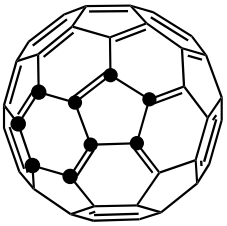
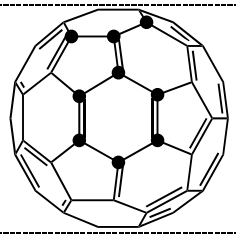
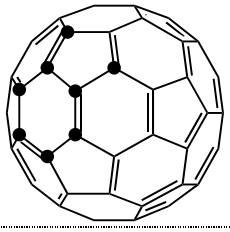
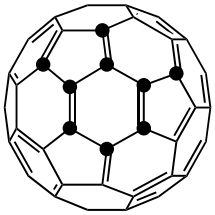
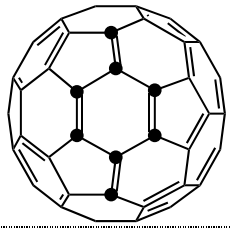
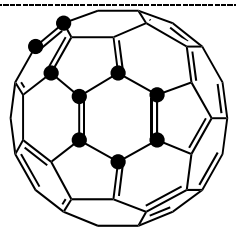
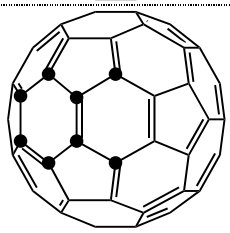
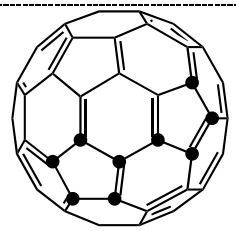
	-458.137883239

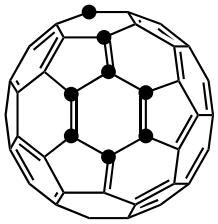
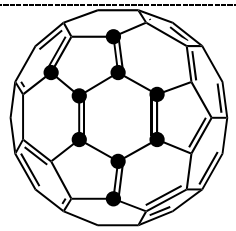
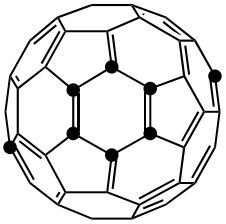
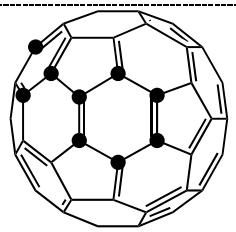
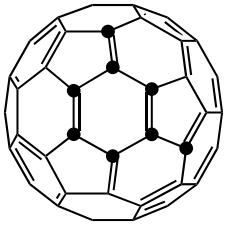
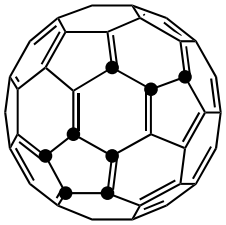
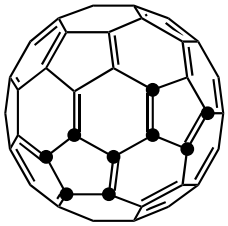
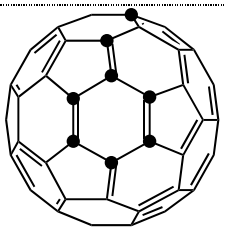
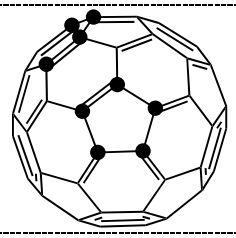
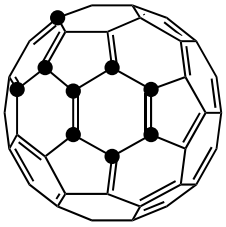
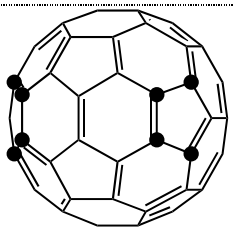
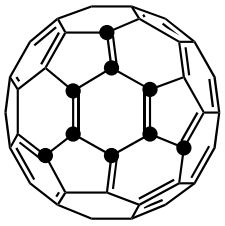
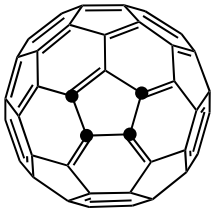
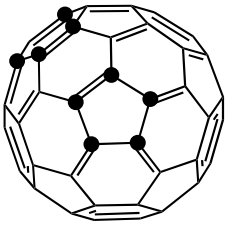
	-490.808424486
	-490.755326572
	-490.698186947
	-490.667432106
	-490.617932 random distribution no C-Ci bond

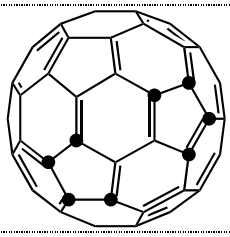
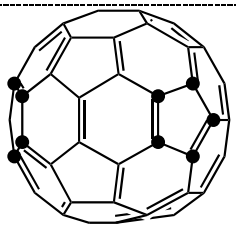
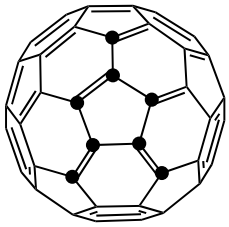
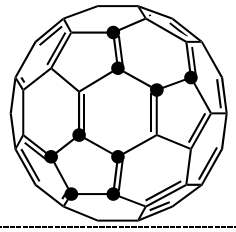
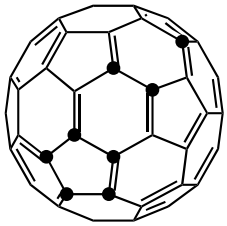
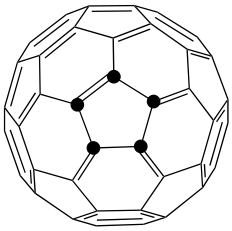
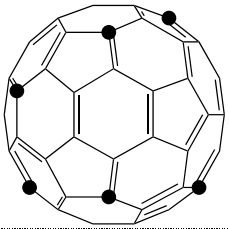
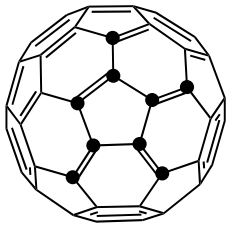
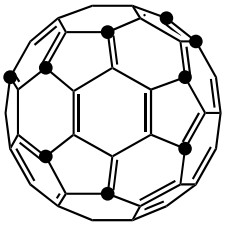
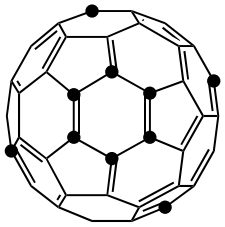
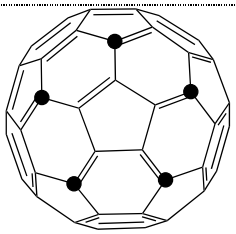
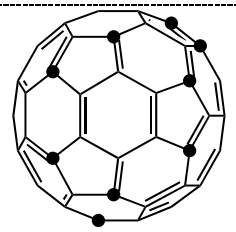
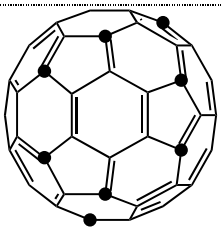
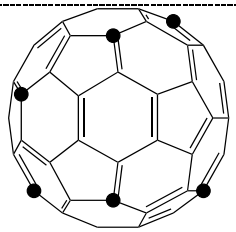
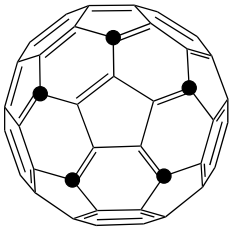
$Bi_{54}C_6$		$Bi_{53}C_7$	
Initial Structure	Total Energy (au)	Initial Structure	Total Energy (au)
	-523.569672850		-556.118058518
	-523.558084124		-556.088482892
	-523.516154		-556.088245716
	-523.503671		-556.064335731
	-523.469932199		-556.058468583
	-523.393803015		-556.055155191
	-523.377131		-556.045206564 other two C atoms at the opposite equivalent positions

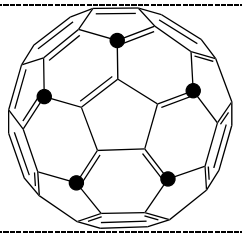
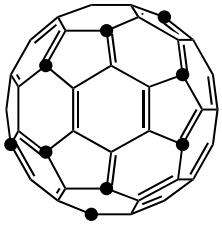
	-523.235188428 one C atom at the opposite equivalent positions
	-523.171573233 partial optimization

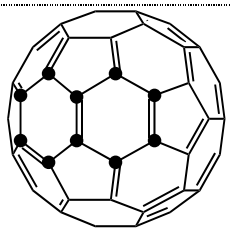
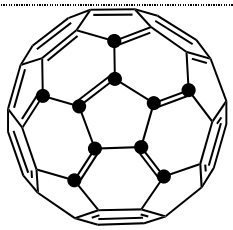
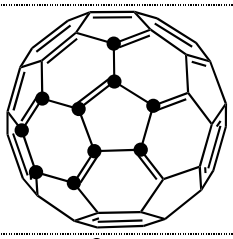
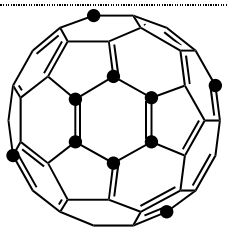
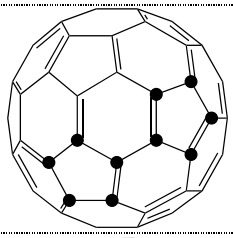
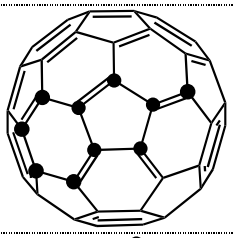
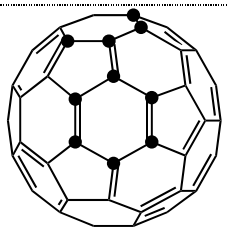
	-556.024442695
	-555.998878643
	-555.997999178 other two C atoms randomly and separated
	-555.996985343
	-555.991562294 other three C atoms at the opposite equivalent positions
	-555.945674 random distribution, no C-C bond
	-555.689007861

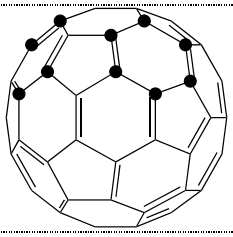
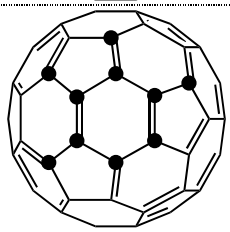
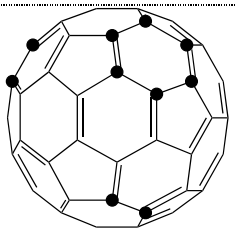
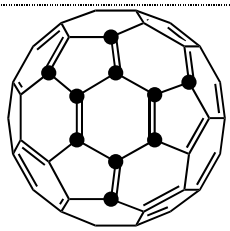
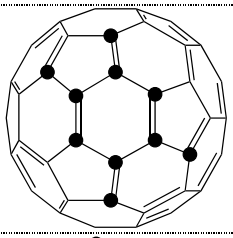
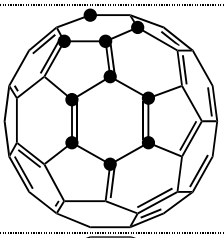
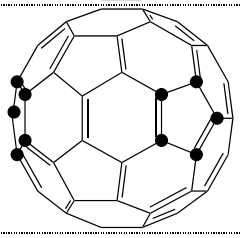
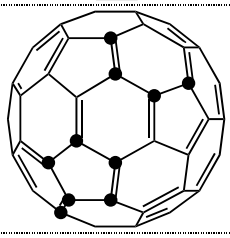
$Bi_{52}C_8$		$Bi_{51}C_9$	
Initial Structure	Total Energy (au)	Initial Structure	Total Energy (au)
	-588.727384959		-621.362777232
	-588.720963936		-621.352397444
	-588.712685236		-621.347286742
	-588.702130238		-621.279332163
	-588.704183838		-621.264695527
	-588.694395		-621.252816041
	-588.686633422		-621.251440226

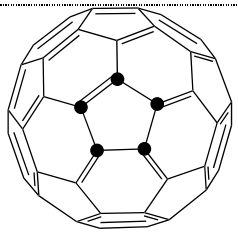
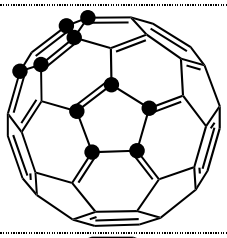
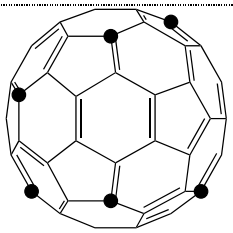
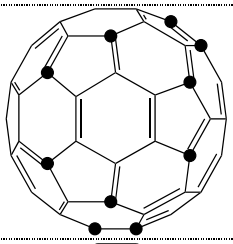
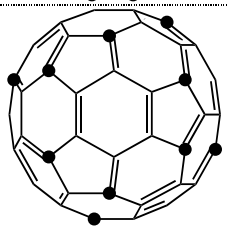
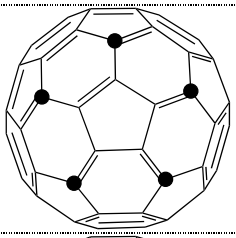
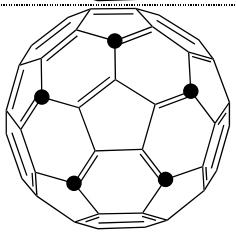
	-588.655710353		-621.246263
	-588.655396758		-621.24199214
	-588.651070624		-621.230845486
	-588.626832774		-621.246242289
	-588.620613079		-621.237830332
	-588.619913543		-621.234207645
	-588.595883847		-621.215139
	-588.593190376 other four C atoms at the opposite equivalent positions		-621.209165067

	-588.591595096		-621.205394585
	-588.5872599		-621.204704914
	-588.575427357		-621.198436088 other four C atoms at the opposite equivalent positions
	-588.523679 random distribution, no C-C bond		-621.171058
	-588.312500089		-621.131124209
	-588.241267956 other three C atoms at the opposite equivalent positions		-620.930519612
	-588.2606126		-620.860804632 random distribution, no C-C bond
			-620.82299062 other four C atoms at the other equivalent positions, not symmetric, not the opposite

	-620.776286156 other four C atoms at the opposite equivalent positions
	-620.775841390

$Bi_{50}C_{10}$	
Initial Structure	Total Energy (au)
	-654.000435539
	-653.958037
	-653.936978455
	-653.9185536
	-653.9000806
	-653.896287452
	-653.884861871

	-653.846745
	-653.845765262
	-653.842540
	-653.8092029
	-653.805825
	-653.803097445
	-653.801438
	-653.795750831

	-653.791565 other five C atoms at the opposite equivalent positions
	-653.782733264
	-653.576746 random distribution, no C-C bond
	-653.459605
	-653.437701
	-653.306977 other five C atoms at the opposite equivalent positions
	-653.302193 other five C atoms at the other equivalent positions, not symmetric, not the opposite