Electronic Supplementary Information for Dalton Transactions

Molecular structures of the 1,6-disubstituted triptycenes $Sb_2(C_6F_4)_3$ and $Bi_2(C_6F_4)_3$ using gas-phase electron diffraction and *ab initio* and DFT calculations

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Table S1 Nozzle-to-film distances (mm), weighting functions (nm^{-1}), scale factors, correlation parameters and electron wavelengths (pm) used in the electron diffraction studies of $Sb_2(C_6F_4)_3$ and $Bi_2(C_6F_4)_3$.

	$Sb_2(C_6F_4)_3$			$Bi_2(C_6F_4)_3$	
Nozzle-to-film distance[a]	94.55	199.49	257.01	199.49	256.88
Δs	2	1	1	1	1
s_{min}	170	100	20	52	20
sw_1	190	120	40	65	40
sw_2	258	176	129	181	60
s_{max}	300	205	150	200	74
Scale factor[b]	0.681(11)	0.793(7)	0.758(5)	0.666(8)	0.560(6)
Correlation parameter	–0.413	0.447	0.482	0.315	–0.153
Electron wavelength	6.013	6.013	6.013	6.013	6.013

[a] Determined by reference to the scattering pattern of benzene. [b] Values in parentheses are the estimated standard deviations.

Table S2 Interatomic distances (r_a), amplitudes of vibration (u_{h1}) and perpendicular corrections (k_{h1}) for the restrained GED structures of $Z_2(C_6F_4)_3$ (Z = Sb, Bi).[a]

	Atom pair	$Sb_2(C_6F_4)_3$				$Bi_2(C_6F_4)_3$			
		r_a/pm	u_{h1}/pm[b]	k_{h1}/pm	Restraint	r_a/pm	u_{h1}/pm[b]	k_{h1}/pm	Restraint
u_1	C(3)–F(8)	133.1(3)	3.6(tied to u_3)	0.1	—	132.1(4)	4.4(2)	0.1	4.2(4)
u_2	C(2)–F(7)	134.7(2)	3.7(tied to u_3)	0.1	—	133.9(4)	4.6(tied to u_1)	0.1	—
u_3	C(3)–C(4)	137.9(3)	3.8(2)	0.1	4.4(4)	139.3(3)	4.7(tied to u_1)	0.1	—
u_4	C(2)–C(1)	138.3(2)	3.9(tied to u_3)	0.1	—	138.5(3)	4.8(tied to u_1)	0.1	—
u_5	C(3)–C(2)	139.0(2)	3.9(tied to u_3)	0.1	—	139.4(2)	4.9(tied to u_1)	0.1	—
u_6	C(1)–C(6)	141.4(4)	4.1(tied to u_3)	0.1	—	139.8(5)	5.0(tied to u_1)	0.1	—
u_7	C(1)–Z(1)	214.4(1)	3.9(2)	0.2	—	223.0(3)	5.8(5)	0.2	—
u_8	C(3)···F(7)	232.5(4)	5.2(tied to u_{10})	–0.1	—	234.2(5)	5.6(2)	–0.1	—
u_9	C(3)···F(9)	235.1(4)	5.2(tied to u_{10})	–0.1	—	234.4(5)	5.6(tied to u_8)	–0.1	—
u_{10}	C(2)···F(8)	235.7(5)	5.2(2)	–0.1	—	235.7(5)	5.7(tied to u_8)	–0.1	—
u_{11}	C(1)···F(7)	237.9(4)	5.0(tied to u_{10})	–0.3	—	237.8(5)	5.5(tied to u_8)	–0.3	—
u_{12}	C(3)···C(5)	238.7(2)	4.6(tied to u_{10})	–0.2	—	241.0(4)	5.0(tied to u_8)	–0.2	—
u_{13}	C(2)···C(6)	240.3(3)	4.7(tied to u_{10})	–0.2	—	240.8(6)	5.1(tied to u_8)	–0.2	—
u_{14}	C(3)···C(1)	242.3(5)	4.6(tied to u_{10})	–0.2	—	240.5(6)	5.0(tied to u_8)	–0.2	—
u_{15}	F(7)···F(8)	265.4(9)	14.7(5)	0.4	—	269.4(9)	11.6(4)	0.4	11.1(11)
u_{16}	F(7)···F(9)	272.0(14)	15.0(tied to u_{15})	–0.2	—	268.9(15)	11.8(tied to u_{15})	–0.2	—
u_{17}	C(2)···C(5)	273.5(5)	8.3(tied to u_{15})	–0.5	—	277.8(10)	6.5(tied to u_{15})	–0.5	—
u_{18}	C(3)···C(6)	279.3(4)	8.5(tied to u_{15})	–0.3	—	277.9(6)	6.7(tied to u_{15})	–0.3	—
u_{19}	C(2)···Z(1)	303.6(3)	9.5(tied to u_{22})	0.1	—	308.2(4)	10.7(tied to u_{22})	0.1	—
u_{20}	C(1)···C(1)′	307.2(3)	12.5(tied to u_{22})	–0.2	—	316.3(5)	14.3(tied to u_{22})	0.4	—
u_{21}	C(1)···Z(2)	315.4(2)	8.6(tied to u_{22})	–0.2	—	323.4(3)	9.6(tied to u_{22})	–0.2	—
u_{22}	F(7)···Z(1)	316.3(4)	14.9(3)	0.4	—	316.1(5)	17.0(4)	–0.2	—
u_{23}	C(1)···C(6)′	338.1(3)	11.8(fixed)	–0.3	—	345.8(5)	11.7(tied to u_{26})	–0.3	—
u_{24}	C(3)···F(10)	358.2(3)	6.1(tied to u_{26})	–0.8	—	361.1(4)	6.0(tied to u_{26})	–0.8	—

u_{25}	C(2)···F(9)	360.4(3)	6.1(tied to u_{26})	–0.8	—	360.7(4)	6.0(tied to u_{26})	–0.7	—
u_{26}	C(1)···F(8)	362.4(4)	6.1(2)	–0.7	—	360.9(5)	6.0(4)	–0.6	—
u_{27}	C(1)···F(10)	364.7(3)	6.1(tied to u_{26})	–0.7	—	364.1(5)	6.0(tied to u_{26})	–0.7	—
u_{28}	Z(1)···Z(2)	380.1(2)	7.9(2)	–0.4	—	393.7(4)	10.5(3)	–0.5	—
u_{29}	C(2)···F(10)	407.5(5)	6.8(tied to u_{31})	–1.1	—	411.2(9)	6.5(fixed)	–1.1	—
u_{30}	C(1)···F(9)	411.7(3)	6.9(tied to u_{31})	–1.1	—	409.3(6)	6.7(fixed)	–1.0	—
u_{31}	C(2)···C(1)′	421.3(3)	15.1(8)	–0.8	—	429.4(4)	15.2(fixed)	–0.9	—
u_{32}	C(3)···Z(1)	436.4(4)	9.7(6)	–0.8	—	441.6(5)	9.7(7)	–0.9	—
u_{33}	C(2)···Z(2)	442.3(2)	9.0(tied to u_{32})	–1.0	—	451.5(4)	8.8(tied to u_{32})	–1.0	—
u_{34}	F(8)···F(10)	466.1(5)	9.8(tied to u_{36})	–1.6	—	467.2(6)	7.9(fixed)	–1.6	—
u_{35}	C(2)···C(6)′	464.3(4)	18.5(tied to u_{36})	–1.2	—	472.1(5)	15.6(fixed)	–1.3	—
u_{36}	C(1)···F(7)′	466.6(4)	23.0(11)	–1.4	—	472.7(4)	19.2(fixed)	–1.4	—
u_{37}	C(3)···Z(2)	492.1(4)	12.7(10)	–1.4	—	499.3(5)	8.2(7)	–1.5	8.1(8)
u_{38}	C(2)···C(2)′	515.4(5)	23.5(tied to u_{42})	–1.6	—	522.0(5)	24.6(tied to u_{42})	–1.6	—
u_{39}	F(7)···F(7)′	526.9(7)	34.6(tied to u_{42})	–0.9	—	529.1(9)	35.7(tied to u_{42})	–1.8	—
u_{40}	C(3)···C(1)′	529.6(4)	18.2(tied to u_{42})	–1.8	—	536.7(6)	19.2(tied to u_{42})	–1.0	—
u_{41}	F(7)···F(10)	541.2(6)	7.6(tied to u_{42})	–1.9	—	544.3(9)	7.6(tied to u_{42})	–1.2	—
u_{42}	F(8)···Z(1)	536.2(5)	11.3(2)	–1.2	—	541.0(5)	11.9(3)	–1.8	—
u_{43}	C(2)···F(7)′	537.9(3)	28.8(tied to u_{42})	–1.7	—	541.9(4)	29.9(tied to u_{42})	–1.8	—
u_{44}	C(1)···F(10)′	542.2(3)	19.7(tied to u_{42})	–1.9	—	546.9(4)	20.6(tied to u_{42})	–1.9	—
u_{45}	F(7)···Z(2)	552.2(3)	9.8(tied to u_{42})	–1.8	—	559.9(4)	10.1(tied to u_{42})	–1.8	—
u_{46}	C(3)···C(6)′	547.4(5)	18.3(tied to u_{42})	–1.9	—	554.3(6)	19.3(tied to u_{42})	–2.0	—
u_{47}	C(2)···C(5)′	582.9(4)	22.6(tied to u_{42})	–2.3	—	590.8(6)	23.6(tied to u_{42})	–2.4	—
u_{48}	F(8)···Z(2)	624.3(3)	9.7(2)	–2.4	8.4(8)	630.3(5)	10.2(6)	–2.5	8.5(9)
u_{49}	C(3)···C(2)′	625.6(6)	29.0(tied to u_{48})	–2.7	—	632.3(7)	25.9(fixed)	–2.8	—
u_{50}	C(1)···F(8)′	642.6(4)	22.2(tied to u_{48})	–2.6	—	649.9(5)	21.0(7)	–2.6	—
u_{51}	C(3)···C(5)′	654.7(5)	28.4(tied to u_{48})	–3.0	—	661.8(6)	26.8(tied to u_{50})	–3.1	—
u_{52}	C(2)···F(10)′	660.4(3)	27.0(tied to u_{48})	–3.1	—	666.3(5)	25.2(tied to u_{50})	–3.2	—
u_{53}	C(3)···F(7)′	658.5(4)	34.6(tied to u_{48})	–3.0	—	663.0(5)	32.3(tied to u_{50})	–3.2	—
u_{54}	C(1)···F(9)′	671.4(4)	21.9(tied to u_{48})	–3.0	—	677.8(5)	20.7(tied to u_{50})	–3.0	—

u_{55}	C(3)···F(10)′	712.4(4)	32.3(10)	–3.6	—	717.1(5)	33.8(tied to u_{59})	–3.8	—
u_{56}	C(3)···C(3)′	722.5(8)	34.6(tied to u_{55})	–3.8	—	728.4(10)	36.6(tied to u_{59})	–3.9	—
u_{57}	C(2)···F(8)′	726.9(5)	33.5(tied to u_{55})	–3.4	—	733.3(6)	35.4(tied to u_{59})	–3.5	—
u_{58}	C(3)···C(4)′	735.4(8)	34.3(tied to u_{55})	–3.9	—	741.4(10)	36.3(tied to u_{59})	–4.1	—
u_{59}	F(7)···F(8)′	744.0(5)	39.8(tied to u_{55})	–3.4	—	748.8(5)	41.7(20)	–3.6	—
u_{60}	F(7)···F(10)′	753.8(6)	27.8(tied to u_{55})	–4.2	—	757.6(8)	29.1(tied to u_{59})	–4.2	—
u_{61}	C(2)···F(9)′	775.8(4)	32.1(tied to u_{55})	–4.2	—	781.9(5)	33.9(tied to u_{59})	–4.3	—
u_{62}	C(3)···F(8)′	824.8(6)	43.8(tied to u_{63})	–4.8	—	830.9(8)	44.1(26)	–5.0	—
u_{63}	F(8)···F(10)′	835.8(3)	38.5(15)	–5.0	—	839.8(4)	38.4(tied to u_{62})	–5.1	—
u_{64}	C(3)···F(9)′	846.8(6)	43.1(tied to u_{63})	–5.3	—	852.7(8)	43.3(tied to u_{62})	–5.4	—
u_{65}	F(8)···F(8)′	918.6(8)	44.7(fixed)	–5.8	—	925.0(8)	45.8(fixed)	–6.0	—
u_{66}	F(8)···F(9)′	957.3(6)	43.2(fixed)	–6.6	—	962.6(8)	44.3(fixed)	–6.8	—

[a] Estimated standard deviations, as obtained in the least squares refinement, are given in parentheses. [b] Amplitudes not refined were fixed at the values obtained using the force field calculated at [RHF/aug-cc-pVQZ-PP/6-31G*] for $Sb_2(C_6F_4)_3$ and $Bi_2(C_6F_4)_3$.

Table S3 Least-squares correlation matrix (×100) for $Sb_2(C_6F_4)_3$.[a]

	p_5	p_9	p_{10}	p_{11}	u_3	u_{10}	u_{28}	u_{32}	u_{36}	u_{37}	k_2	k_3
p_1	–86	–67	–56		–75							
p_2				–75								
p_5					80							
p_7			52			61						
p_9			71									
u_3						68						61
u_7						69						59
u_{10}												69
u_{26}							69					
u_{31}								62	56			
u_{32}									79			
u_{36}										69		
k_1											51	
k_2												62

[a] Only elements with absolute values ≥ 50% are shown; k_1, k_2 and k_3 are scale factors.

Table S4 Least-squares correlation matrix (×100) for $Bi_2(C_6F_4)_3$.[a]

	p_5	p_7	p_{10}	p_{11}	u_1	u_{59}
p_1	–87	–51			–60	
p_2				–58		
p_5					64	
p_9			65			
u_{50}						51

[a] Only elements with absolute values ≥ 50% are shown.

Figure S1 Experimental and difference (experimental – theoretical) molecular-scattering intensities for $Sb_2(C_6F_4)_3$.

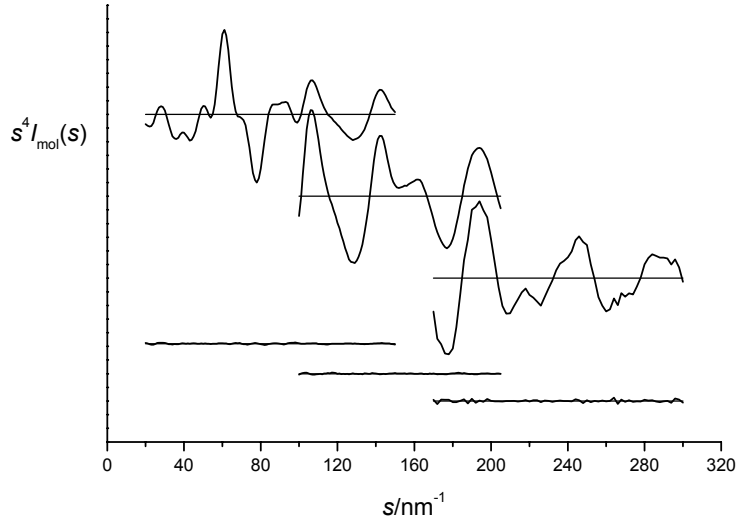

Figure S2 Experimental and difference (experimental – theoretical) molecular-scattering intensities for $Bi_2(C_6F_4)_3$.

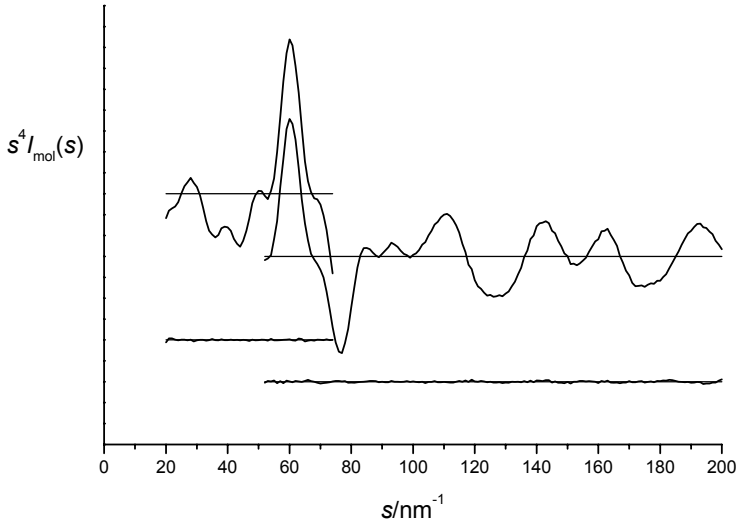

Table S5 Experimental (GED) coordinates for $Sb_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2028	0.6926
C(2)	0.0000	2.9899	1.3693
C(3)	0.0000	1.7772	0.7043
C(4)	0.0000	1.7772	–0.7043
C(5)	0.0000	2.9899	–1.3693
C(6)	0.0000	4.2028	–0.6926
F(7)	0.0000	5.3485	1.3640
F(8)	0.0000	3.0618	2.7161
F(9)	0.0000	3.0618	–2.7161
F(10)	0.0000	5.3485	–1.3640
C(1)′	–3.6398	–2.1014	0.6926
C(2)′	–2.5894	–1.4950	1.3693
C(3)′	–1.5391	–0.8886	0.7043
C(4)′	–1.5391	–0.8886	–0.7043
C(5)′	–2.5894	–1.4950	–1.3693
C(6)′	–3.6398	–2.1014	–0.6926
F(7)′	–4.6319	–2.6742	1.3640
F(8)′	–2.6516	–1.5309	2.7161
F(9)′	–2.6516	–1.5309	–2.7161
F(10)′	–4.6319	–2.6742	–1.3640
C(1)″	3.6398	–2.1014	0.6926
C(2)″	2.5894	–1.4950	1.3693
C(3)″	1.5391	–0.8886	0.7043
C(4)″	1.5391	–0.8886	–0.7043
C(5)″	2.5894	–1.4950	–1.3693
C(6)″	3.6398	–2.1014	–0.6926
F(7)″	4.6319	–2.6742	1.3640
F(8)″	2.6516	–1.5309	2.7161
F(9)″	2.6516	–1.5309	–2.7161
F(10)″	4.6319	–2.6742	–1.3640
Sb(1)	0.0000	0.0000	1.9029
Sb(2)	0.0000	0.0000	–1.9029

[a] All coordinates in Å.

Table S6 Experimental (GED) coordinates for $Bi_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2386	0.6966
C(2)	0.0000	3.0298	1.3921
C(3)	0.0000	1.8304	0.6994
C(4)	0.0000	1.8304	–0.6994
C(5)	0.0000	3.0298	–1.3921
C(6)	0.0000	4.2386	–0.6966
F(7)	0.0000	5.3880	1.3481
F(8)	0.0000	3.0744	2.7309
F(9)	0.0000	3.0744	–2.7309
F(10)	0.0000	5.3880	–1.3481
C(1)′	3.6707	–2.1193	0.6966
C(2)′	–2.6239	–1.5149	1.3921
C(3)′	–1.5852	–0.9152	0.6994
C(4)′	–1.5852	–0.9152	–0.6994
C(5)′	–2.6239	–1.5149	–1.3921
C(6)′	–3.6707	–2.1193	–0.6966
F(7)′	–4.6661	–2.6940	1.3481
F(8)′	–2.6625	–1.5372	2.7309
F(9)′	–2.6625	–1.5372	–2.7309
F(10)′	–4.6661	–2.6940	–1.3481
C(1)″	3.6707	–2.1193	0.6966
C(2)″	2.6239	–1.5149	1.3921
C(3)″	1.5852	–0.9152	0.6994
C(4)″	1.5852	–0.9152	–0.6994
C(5)″	2.6239	–1.5149	–1.3921
C(6)″	3.6707	–2.1193	–0.6966
F(7)″	4.6661	–2.6940	1.3481
F(8)″	2.6625	–1.5372	2.7309
F(9)″	2.6625	–1.5372	–2.7309
F(10)″	4.6661	–2.6940	–1.3481
Bi(1)	0.0000	0.0000	1.9722
Bi(2)	0.0000	0.0000	–1.9722

[a] All coordinates in Å.

Table S7 Calculated [MP2/LanL2DZ/6-311G*] coordinates for $Sb_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2340	0.6958
C(2)	0.0000	3.0149	1.3756
C(3)	0.0000	1.7943	0.7046
C(4)	0.0000	1.7943	–0.7046
C(5)	0.0000	3.0149	–1.3756
C(6)	0.0000	4.2340	–0.6958
F(7)	0.0000	5.3878	1.3598
F(8)	0.0000	3.0692	2.7204
F(9)	0.0000	3.0692	–2.7204
F(10)	0.0000	5.3878	–1.3598
C(1′)	–3.6668	–2.1170	0.6958
C(2′)	–2.6110	–1.5075	1.3756
C(3′)	–1.5539	–0.8971	0.7046
C(4′)	–1.5539	–0.8971	–0.7046
C(5′)	–2.6110	–1.5075	–1.3756
C(6′)	–3.6668	–2.1170	–0.6958
F(7′)	–4.6659	–2.6939	1.3598
F(8′)	–2.6580	–1.5346	2.7204
F(9′)	–2.6580	–1.5346	–2.7204
F(10′)	–4.6659	–2.6939	–1.3598
C(1″)	3.6668	–2.1170	0.6958
C(2″)	2.6110	–1.5075	1.3756
C(3″)	1.5539	–0.8971	0.7046
C(4″)	1.5539	–0.8971	–0.7046
C(5″)	2.6110	–1.5075	–1.3756
C(6″)	3.6668	–2.1170	–0.6958
F(7″)	4.6659	–2.6939	1.3598
F(8″)	2.6580	–1.5346	2.7204
F(9″)	2.6580	–1.5346	–2.7204
F(10″)	4.6659	–2.6939	–1.3598
Sb(1)	0.0000	0.0000	1.9271
Sb(2)	0.0000	0.0000	–1.9271

[a] All coordinates in Å.
Energy = –1890.60154 Hartrees (corrected for ZPE).

Table S8 Calculated [MP2/aug-cc-pVQZ-PP/6-311G*] coordinates for $Sb_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	1.7667	0.7040
C(2)	0.0000	2.9823	1.3820
C(3)	0.0000	4.2004	0.6979
C(4)	0.0000	4.2004	–0.6979
C(5)	0.0000	2.9823	–1.3820
C(6)	0.0000	1.7667	–0.7040
F(7)	0.0000	3.0162	2.7267
F(8)	0.0000	5.3553	1.3589
F(9)	0.0000	5.3553	–1.3589
F(10)	0.0000	3.0162	–2.7267
C(1′)	–3.6376	–2.1002	–0.6979
C(2′)	–3.6376	–2.1002	0.6979
C(3′)	–2.5828	–1.4912	1.3820
C(4′)	–1.5300	–0.8833	0.7040
C(5′)	–1.5300	–0.8833	–0.7040
C(6′)	–2.5828	–1.4912	–1.3820
F(7′)	–4.6378	–2.6777	1.3589
F(8′)	–2.6121	–1.5081	2.7267
F(9′)	–2.6121	–1.5081	–2.7267
F(10′)	–4.6378	–2.6777	–1.3589
C(1″)	2.5828	–1.4912	1.3820
C(2″)	1.5300	–0.8833	0.7040
C(3″)	1.5300	–0.8833	–0.7040
C(4″)	2.5828	–1.4912	–1.3820
C(5″)	3.6376	–2.1002	–0.6979
C(6″)	3.6376	–2.1002	0.6979
F(7″)	4.6378	–2.6777	1.3589
F(8″)	2.6121	–1.5081	2.7267
F(9″)	2.6121	–1.5081	–2.7267
F(10″)	4.6378	–2.6777	–1.3589
Sb(1)	0.0000	0.0000	1.9006
Sb(2)	0.0000	0.0000	–1.9006

[a] All coordinates in Å.
Energy = –2353.72102 Hartrees (corrected for ZPE).

Table S9 Calculated [B3PW91/LanL2DZ/6-311G*] coordinates for $Sb_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2240	0.6932
C(2)	0.0000	3.0097	1.3718
C(3)	0.0000	1.8000	0.7003
C(4)	0.0000	1.8000	–0.7003
C(5)	0.0000	3.0097	–1.3718
C(6)	0.0000	4.2240	–0.6932
F(7)	0.0000	5.3750	1.3561
F(8)	0.0000	3.0531	2.7144
F(9)	0.0000	3.0531	–2.7144
F(10)	0.0000	5.3750	–1.3561
C(1′)	–3.6580	–2.1120	0.6932
C(2′)	–2.6065	–1.5048	1.3718
C(3′)	–1.5589	–0.9000	0.7003
C(4′)	–1.5589	–0.9000	–0.7003
C(5′)	–2.6065	–1.5048	–1.3718
C(6′)	–3.6580	–2.1120	–0.6932
F(7′)	–4.6549	–2.6875	1.3561
F(8′)	–2.6441	–1.5266	2.7144
F(9′)	–2.6441	–1.5266	–2.7144
F(10′)	–4.6549	–2.6875	–1.3561
C(1″)	3.6580	–2.1120	0.6932
C(2″)	2.6065	–1.5048	1.3718
C(3″)	1.5589	–0.9000	0.7003
C(4″)	1.5589	–0.9000	–0.7003
C(5″)	2.6065	–1.5048	–1.3718
C(6″)	3.6580	–2.1120	–0.6932
F(7″)	4.6549	–2.6875	1.3561
F(8″)	2.6441	–1.5266	2.7144
F(9″)	2.6441	–1.5266	–2.7144
F(10″)	4.6549	–2.6875	–1.3561
Sb(1)	0.0000	0.0000	1.9099
Sb(2)	0.0000	0.0000	–1.9099

[a] All coordinates in Å.
Energy = –2364.43391 Hartrees (corrected for ZPE).

Table S10 Calculated [B3PW91/aug-cc-pVQZ-PP/6-311G*] coordinates for $Sb_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2236	0.6933
C(2)	0.0000	3.0091	1.3708
C(3)	0.0000	1.7987	0.7009
C(4)	0.0000	1.7987	–0.7009
C(5)	0.0000	3.0091	–1.3708
C(6)	0.0000	4.2236	–0.6933
F(7)	0.0000	5.3743	1.3563
F(8)	0.0000	3.0518	2.7140
F(9)	0.0000	3.0518	–2.7140
F(10)	0.0000	5.3743	–1.3563
C(1′)	–3.6578	–2.1118	0.6933
C(2′)	–2.6059	–1.5045	1.3708
C(3′)	–1.5577	–0.8993	0.7009
C(4′)	–1.5577	–0.8993	–0.7009
C(5′)	–2.6059	–1.5045	–1.3708
C(6′)	–3.6578	–2.1118	–0.6933
F(7′)	–4.6543	–2.6872	1.3563
F(8′)	–2.6429	–1.5259	2.7140
F(9′)	–2.6429	–1.5259	–2.7140
F(10′)	–4.6543	–2.6872	–1.3563
C(1″)	3.6578	–2.1118	0.6933
C(2″)	2.6059	–1.5045	1.3708
C(3″)	1.5577	–0.8993	0.7009
C(4″)	1.5577	–0.8993	–0.7009
C(5″)	2.6059	–1.5045	–1.3708
C(6″)	3.6578	–2.1118	–0.6933
F(7″)	4.6543	–2.6872	1.3563
F(8″)	2.6429	–1.5259	2.7140
F(9″)	2.6429	–1.5259	–2.7140
F(10″)	4.6543	–2.6872	–1.3563
Sb(1)	0.0000	0.0000	1.9097
Sb(2)	0.0000	0.0000	–1.9097

[a] All coordinates in Å.
Energy = –2364.43391 Hartrees (corrected for ZPE).

Table S11 Calculated [B3LYP/LanL2DZ/6-311G*] coordinates for $Sb_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2462	0.6932
C(2)	0.0000	3.0303	1.3714
C(3)	0.0000	1.8173	0.7021
C(4)	0.0000	1.8173	–0.7021
C(5)	0.0000	3.0303	–1.3714
C(6)	0.0000	4.2462	–0.6932
F(7)	0.0000	5.4011	1.3610
F(8)	0.0000	3.0769	2.7205
F(9)	0.0000	3.0769	–2.7205
F(10)	0.0000	5.4011	–1.3610
C(1′)	–3.6773	–2.1231	0.6932
C(2′)	–2.6243	–1.5151	1.3714
C(3′)	–1.5738	–0.9086	0.7021
C(4′)	–1.5738	–0.9086	–0.7021
C(5′)	–2.6243	–1.5151	–1.3714
C(6′)	–3.6773	–2.1231	–0.6932
F(7′)	–4.6775	–2.7006	1.3610
F(8′)	–2.6647	–1.5384	2.7205
F(9′)	–2.6647	–1.5384	–2.7205
F(10′)	–4.6775	–2.7006	–1.3610
C(1″)	3.6773	–2.1231	0.6932
C(2″)	2.6243	–1.5151	1.3714
C(3″)	1.5738	–0.9086	0.7021
C(4″)	1.5738	–0.9086	–0.7021
C(5″)	2.6243	–1.5151	–1.3714
C(6″)	3.6773	–2.1231	–0.6932
F(7″)	4.6775	–2.7006	1.3610
F(8″)	2.6647	–1.5384	2.7205
F(9″)	2.6647	–1.5384	–2.7205
F(10″)	4.6775	–2.7006	–1.3610
Sb(1)	0.0000	0.0000	1.9279
Sb(2)	0.0000	0.0000	–1.9279

[a] All coordinates in Å.
Energy = –1895.18126 Hartrees (corrected for ZPE).

Table S12 Calculated [B3LYP/aug-cc-pVQZ-PP/6-311G*] coordinates for $Sb_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2387	0.6940
C(2)	0.0000	3.0221	1.3704
C(3)	0.0000	1.8100	0.7016
C(4)	0.0000	1.8100	–0.7016
C(5)	0.0000	3.0221	–1.3704
C(6)	0.0000	4.2387	–0.6940
F(7)	0.0000	5.3939	1.3613
F(8)	0.0000	3.0625	2.7220
F(9)	0.0000	3.0625	–2.7220
F(10)	0.0000	5.3939	–1.3613
C(1′)	–3.6708	–2.1193	0.6940
C(2′)	–2.6172	–1.5111	1.3704
C(3′)	–1.5675	–0.9050	0.7016
C(4′)	–1.5675	–0.9050	–0.7016
C(5′)	–2.6172	–1.5111	–1.3704
C(6′)	–3.6708	–2.1193	–0.6940
F(7′)	–4.6713	–2.6970	1.3613
F(8′)	–2.6522	–1.5312	2.7220
F(9′)	–2.6522	–1.5312	–2.7220
F(10′)	–4.6713	–2.6970	–1.3613
C(1″)	3.6708	–2.1193	0.6940
C(2″)	2.6172	–1.5111	1.3704
C(3″)	1.5675	–0.9050	0.7016
C(4″)	1.5675	–0.9050	–0.7016
C(5″)	2.6172	–1.5111	–1.3704
C(6″)	3.6708	–2.1193	–0.6940
F(7″)	4.6713	–2.6970	1.3613
F(8″)	2.6522	–1.5312	2.7220
F(9″)	2.6522	–1.5312	–2.7220
F(10″)	4.6713	–2.6970	–1.3613
Sb(1)	0.0000	0.0000	1.9244
Sb(2)	0.0000	0.0000	–1.9244

[a] All coordinates in Å.
Energy = –2365.08049 Hartrees (corrected for ZPE).

Table S13 Calculated [BLYP/LanL2DZ/6-311G*] coordinates for $Sb_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2799	0.6992
C(2)	0.0000	3.0539	1.3826
C(3)	0.0000	1.8324	0.7066
C(4)	0.0000	1.8324	–0.7066
C(5)	0.0000	3.0539	–1.3826
C(6)	0.0000	4.2799	–0.6992
F(7)	0.0000	5.4504	1.3739
F(8)	0.0000	3.1013	2.7493
F(9)	0.0000	3.1013	–2.7493
F(10)	0.0000	5.4504	–1.3739
C(1′)	–3.7065	–2.1399	0.6992
C(2′)	–2.6448	–1.5270	1.3826
C(3′)	–1.5869	–0.9162	0.7066
C(4′)	–1.5869	–0.9162	–0.7066
C(5′)	–2.6448	–1.5270	–1.3826
C(6′)	–3.7065	–2.1399	–0.6992
F(7′)	–4.7202	–2.7252	1.3739
F(8′)	–2.6858	–1.5506	2.7493
F(9′)	–2.6858	–1.5506	–2.7493
F(10′)	–4.7202	–2.7252	–1.3739
C(1″)	3.7065	–2.1399	0.6992
C(2″)	2.6448	–1.5270	1.3826
C(3″)	1.5869	–0.9162	0.7066
C(4″)	1.5869	–0.9162	–0.7066
C(5″)	2.6448	–1.5270	–1.3826
C(6″)	3.7065	–2.1399	–0.6992
F(7″)	4.7202	–2.7252	1.3739
F(8″)	2.6858	–1.5506	2.7493
F(9″)	2.6858	–1.5506	–2.7493
F(10″)	4.7202	–2.7252	–1.3739
Sb(1)	0.0000	0.0000	1.9452
Sb(2)	0.0000	0.0000	–1.9452

[a] All coordinates in Å.
Energy = –1894.87117 Hartrees (corrected for ZPE).

Table S14 Calculated [BLYP/aug-cc-pVQZ-PP/6-311G*] coordinates for $Sb_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2760	0.7001
C(2)	0.0000	3.0491	1.3807
C(3)	0.0000	1.8290	0.7059
C(4)	0.0000	1.8290	–0.7059
C(5)	0.0000	3.0491	–1.3807
C(6)	0.0000	4.2760	–0.7001
F(7)	0.0000	5.4468	1.3743
F(8)	0.0000	3.0876	2.7515
F(9)	0.0000	3.0876	–2.7515
F(10)	0.0000	5.4468	–1.3743
C(1′)	–3.7031	–2.1380	0.7001
C(2′)	–2.6406	–1.5245	1.3807
C(3′)	–1.5839	–0.9145	0.7059
C(4′)	–1.5839	–0.9145	–0.7059
C(5′)	–2.6406	–1.5245	–1.3807
C(6′)	–3.7031	–2.1380	–0.7001
F(7′)	–4.7171	–2.7234	1.3743
F(8′)	–2.6739	–1.5438	2.7515
F(9′)	–2.6739	–1.5438	–2.7515
F(10′)	–4.7171	–2.7234	–1.3743
C(1″)	3.7031	–2.1380	0.7001
C(2″)	2.6406	–1.5245	1.3807
C(3″)	1.5839	–0.9145	0.7059
C(4″)	1.5839	–0.9145	–0.7059
C(5″)	2.6406	–1.5245	–1.3807
C(6″)	3.7031	–2.1380	–0.7001
F(7″)	4.7171	–2.7234	1.3743
F(8″)	2.6739	–1.5438	2.7515
F(9″)	2.6739	–1.5438	–2.7515
F(10″)	4.7171	–2.7234	–1.3743
Sb(1)	0.0000	0.0000	1.9483
Sb(2)	0.0000	0.0000	–1.9483

[a] All coordinates in Å.
Energy = –2364.56211 Hartrees (corrected for ZPE).

Table S15 Calculated [MP2/LanL2DZ/6-311G*] coordinates for $Bi_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2777	0.6963
C(2)	0.0000	3.0576	1.3733
C(3)	0.0000	1.8377	0.7032
C(4)	0.0000	1.8377	–0.7032
C(5)	0.0000	3.0576	–1.3733
C(6)	0.0000	4.2777	–0.6963
F(7)	0.0000	5.4329	1.3602
F(8)	0.0000	3.1060	2.7224
F(9)	0.0000	3.1060	–2.7224
F(10)	0.0000	5.4329	–1.3602
C(1′)	–3.7046	–2.1389	0.6963
C(2′)	–2.6479	–1.5288	1.3733
C(3′)	–1.5915	–0.9188	0.7032
C(4′)	–1.5915	–0.9188	–0.7032
C(5′)	–2.6479	–1.5288	–1.3733
C(6′)	–3.7046	–2.1389	–0.6963
F(7′)	–4.7051	–2.7165	1.3602
F(8′)	–2.6899	–1.5530	2.7224
F(9′)	–2.6899	–1.5530	–2.7224
F(10′)	–4.7051	–2.7165	–1.3602
C(1″)	3.7046	–2.1389	0.6963
C(2″)	2.6479	–1.5288	1.3733
C(3″)	1.5915	–0.9188	0.7032
C(4″)	1.5915	–0.9188	–0.7032
C(5″)	2.6479	–1.5288	–1.3733
C(6″)	3.7046	–2.1389	–0.6963
F(7″)	4.7051	–2.7165	1.3602
F(8″)	2.6899	–1.5530	2.7224
F(9″)	2.6899	–1.5530	–2.7224
F(10″)	4.7051	–2.7165	–1.3602
Bi(1)	0.0000	0.0000	1.9912
Bi(2)	0.0000	0.0000	–1.9912

[a] All coordinates in Å.

Energy = –1890.67381 Hartrees (corrected for ZPE)

Table S16 Calculated [MP2/aug-cc-pVTZ-PP/6-311G*] coordinates for $Bi_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2594	0.6980
C(2)	0.0000	3.0414	1.3806
C(3)	0.0000	1.8267	0.7016
C(4)	0.0000	1.8267	–0.7016
C(5)	0.0000	3.0414	–1.3806
C(6)	0.0000	4.2594	–0.6980
F(7)	0.0000	5.4161	1.3583
F(8)	0.0000	3.0773	2.7274
F(9)	0.0000	3.0773	–2.7274
F(10)	0.0000	5.4161	–1.3583
C(1)′	–3.6888	–2.1297	0.6980
C(2)′	–2.6339	–1.5207	1.3806
C(3)′	–1.5820	–0.9133	0.7016
C(4)′	–1.5820	–0.9133	–0.7016
C(5)′	–2.6339	–1.5207	–1.3806
C(6)′	–3.6888	–2.1297	–0.6980
F(7)′	–4.6905	–2.7081	1.3583
F(8)′	–2.6651	–1.5387	2.7274
F(9)′	–2.6651	–1.5387	–2.7274
F(10)′	–4.6905	–2.7081	–1.3583
C(1)″	3.6888	–2.1297	0.6980
C(2)″	2.6339	–1.5207	1.3806
C(3)″	1.5820	–0.9133	0.7016
C(4)″	1.5820	–0.9133	–0.7016
C(5)″	2.6339	–1.5207	–1.3806
C(6)″	3.6888	–2.1297	–0.6980
F(7)″	4.6905	–2.7081	1.3583
F(8)″	2.6651	–1.5387	2.7274
F(9)″	2.6651	–1.5387	–2.7274
F(10)″	4.6905	–2.7081	–1.3583
Bi(1)	0.0000	0.0000	1.9793
Bi(2)	0.0000	0.0000	–1.9793

[a] All coordinates in Å.

Energy = –2307.87495 Hartrees (corrected for ZPE)

Table S17 Calculated [B3PW91/LanL2DZ/6-311G*] coordinates for $Bi_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2823	0.6933
C(2)	0.0000	3.0668	1.3689
C(3)	0.0000	1.8572	0.6989
C(4)	0.0000	1.8572	–0.6989
C(5)	0.0000	3.0668	–1.3689
C(6)	0.0000	4.2823	–0.6933
F(7)	0.0000	5.4335	1.3578
F(8)	0.0000	3.1078	2.7148
F(9)	0.0000	3.1078	–2.7148
F(10)	0.0000	5.4335	–1.3578
C(1′)	–3.7086	–2.1412	0.6933
C(2′)	–2.6560	–1.5334	1.3689
C(3′)	–1.6083	–0.9286	0.6989
C(4′)	–1.6083	–0.9286	–0.6989
C(5′)	–2.6560	–1.5334	–1.3689
C(6′)	–3.7086	–2.1412	–0.6933
F(7′)	–4.7056	–2.7168	1.3578
F(8′)	–2.6914	–1.5539	2.7148
F(9′)	–2.6914	–1.5539	–2.7148
F(10′)	–4.7056	–2.7168	–1.3578
C(1″)	3.7086	–2.1412	0.6933
C(2″)	2.6560	–1.5334	1.3689
C(3″)	1.6083	–0.9286	0.6989
C(4″)	1.6083	–0.9286	–0.6989
C(5″)	2.6560	–1.5334	–1.3689
C(6″)	3.7086	–2.1412	–0.6933
F(7″)	4.7056	–2.7168	1.3578
F(8″)	2.6914	–1.5539	2.7148
F(9″)	2.6914	–1.5539	–2.7148
F(10″)	4.7056	–2.7168	–1.3578
Bi(1)	0.0000	0.0000	1.9807
Bi(2)	0.0000	0.0000	–1.9807

[a] All coordinates in Å.
Energy = –1894.58547 Hartrees (corrected for ZPE)

Table S18 Calculated [B3PW91/aug-cc-pVTZ-PP/6-311G*] coordinates for $Bi_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2841	0.6938
C(2)	0.0000	3.0690	1.3694
C(3)	0.0000	1.8610	0.6982
C(4)	0.0000	1.8610	–0.6982
C(5)	0.0000	3.0690	–1.3694
C(6)	0.0000	4.2841	–0.6938
F(7)	0.0000	5.4367	1.3562
F(8)	0.0000	3.1058	2.7164
F(9)	0.0000	3.1058	–2.7164
F(10)	0.0000	5.4367	–1.3562
C(1′)	–3.7147	–2.1409	0.6938
C(2′)	–2.6612	–1.5352	1.3692
C(3′)	–1.6140	–0.9330	0.6981
C(4′)	–1.6140	–0.9330	–0.6981
C(5′)	–2.6612	–1.5352	–1.3692
C(6′)	–3.7147	–2.1409	–0.6938
F(7′)	–4.7140	–2.7149	1.3567
F(8′)	–2.6933	–1.5532	2.7162
F(9′)	–2.6933	–1.5532	–2.7162
F(10′)	–4.7140	–2.7149	–1.3567
C(1″)	3.7147	–2.1409	0.6938
C(2″)	2.6612	–1.5352	1.3692
C(3″)	1.6140	–0.9330	0.6981
C(4″)	1.6140	–0.9330	–0.6981
C(5″)	2.6612	–1.5352	–1.3692
C(6″)	3.7147	–2.1409	–0.6938
F(7″)	4.7140	–2.7149	1.3567
F(8″)	2.6933	–1.5532	2.7162
F(9″)	2.6933	–1.5532	–2.7162
F(10″)	4.7140	–2.7149	–1.3567
Bi(1)	0.0000	0.0000	1.9882
Bi(2)	0.0000	0.0000	–1.9882

[a] All coordinates in Å.

Energy = –2313.03393 Hartrees (corrected for ZPE)

Table S19 Calculated [B3LYP/LanL2DZ/6-311G*] coordinates for $Bi_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.2929	0.6939
C(2)	0.0000	3.0759	1.3700
C(3)	0.0000	1.8641	0.7003
C(4)	0.0000	1.8641	–0.7003
C(5)	0.0000	3.0759	–1.3700
C(6)	0.0000	4.2929	–0.6939
F(7)	0.0000	5.4495	1.3614
F(8)	0.0000	3.1166	2.7225
F(9)	0.0000	3.1166	–2.7225
F(10)	0.0000	5.4495	–1.3614
C(1′)	–3.7178	–2.1465	0.6939
C(2′)	–2.6638	–1.5379	1.3700
C(3′)	–1.6144	–0.9321	0.7003
C(4′)	–1.6144	–0.9321	–0.7003
C(5′)	–2.6638	–1.5379	–1.3700
C(6′)	–3.7178	–2.1465	–0.6939
F(7′)	–4.7194	–2.7247	1.3614
F(8′)	–2.6990	–1.5583	2.7225
F(9′)	–2.6990	–1.5583	–2.7225
F(10′)	–4.7194	–2.7247	–1.3614
C(1″)	3.7178	–2.1465	0.6939
C(2″)	2.6638	–1.5379	1.3700
C(3″)	1.6144	–0.9321	0.7003
C(4″)	1.6144	–0.9321	–0.7003
C(5″)	2.6638	–1.5379	–1.3700
C(6″)	3.7178	–2.1465	–0.6939
F(7″)	4.7194	–2.7247	1.3614
F(8″)	2.6990	–1.5583	2.7225
F(9″)	2.6990	–1.5583	–2.7225
F(10″)	4.7194	–2.7247	–1.3614
Bi(1)	0.0000	0.0000	1.9857
Bi(2)	0.0000	0.0000	–1.9857

[a] All coordinates in Å.

Energy = –1895.26698 Hartrees (corrected for ZPE)

Table S20 Calculated [B3LYP/aug-cc-pVTZ-PP/6-311G*] coordinates for $Bi_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.3062	0.6945
C(2)	0.0000	3.0892	1.3696
C(3)	0.0000	1.8790	0.6993
C(4)	0.0000	1.8790	–0.6993
C(5)	0.0000	3.0892	–1.3696
C(6)	0.0000	4.3062	–0.6945
F(7)	0.0000	5.4635	1.3610
F(8)	0.0000	3.1255	2.7238
F(9)	0.0000	3.1255	–2.7238
F(10)	0.0000	5.4635	–1.3610
C(1)′	–3.7293	–2.1531	0.6945
C(2)′	–2.6753	–1.5446	1.3696
C(3)′	–1.6273	–0.9395	0.6993
C(4)′	–1.6273	–0.9395	–0.6993
C(5)′	–2.6753	–1.5446	–1.3696
C(6)′	–3.7293	–2.1531	–0.6945
F(7)′	–4.7315	–2.7317	1.3610
F(8)′	–2.7067	–1.5627	2.7238
F(9)′	–2.7067	–1.5627	–2.7238
F(10)′	–4.7315	–2.7317	–1.3610
C(1)″	3.7293	–2.1531	0.6945
C(2)″	2.6753	–1.5446	1.3696
C(3)″	1.6273	–0.9395	0.6993
C(4)″	1.6273	–0.9395	–0.6993
C(5)″	2.6753	–1.5446	–1.3696
C(6)″	3.7293	–2.1531	–0.6945
F(7)″	4.7315	–2.7317	1.3610
F(8)″	2.7067	–1.5627	2.7238
F(9)″	2.7067	–1.5627	–2.7238
F(10)″	4.7315	–2.7317	–1.3610
Bi(1)	0.0000	0.0000	2.0010
Bi(2)	0.0000	0.0000	–2.0010

[a] All coordinates in Å.

Energy = –2313.80950 Hartrees (corrected for ZPE)

Table S21 Calculated [BLYP/LanL2DZ/6-311G*] coordinates for $Bi_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.3264	0.6997
C(2)	0.0000	3.0996	1.3807
C(3)	0.0000	1.8796	0.7049
C(4)	0.0000	1.8796	–0.7049
C(5)	0.0000	3.0996	–1.3807
C(6)	0.0000	4.3264	–0.6997
F(7)	0.0000	5.4989	1.3741
F(8)	0.0000	3.1406	2.7518
F(9)	0.0000	3.1406	–2.7518
F(10)	0.0000	5.4989	–1.3741
C(1)′	–3.7467	–2.1632	0.6997
C(2)′	–2.6843	–1.5498	1.3807
C(3)′	–1.6278	–0.9398	0.7049
C(4)′	–1.6278	–0.9398	–0.7049
C(5)′	–2.6843	–1.5498	–1.3807
C(6)′	–3.7467	–2.1632	–0.6997
F(7)′	–4.7621	–2.7494	1.3741
F(8)′	–2.7198	–1.5703	2.7518
F(9)′	–2.7198	–1.5703	–2.7518
F(10)′	–4.7621	–2.7494	–1.3741
C(1)″	3.7467	–2.1632	0.6997
C(2)″	2.6843	–1.5498	1.3807
C(3)″	1.6278	–0.9398	0.7049
C(4)″	1.6278	–0.9398	–0.7049
C(5)″	2.6843	–1.5498	–1.3807
C(6)″	3.7467	–2.1632	–0.6997
F(7)″	4.7621	–2.7494	1.3741
F(8)″	2.7198	–1.5703	2.7518
F(9)″	2.7198	–1.5703	–2.7518
F(10)″	4.7621	–2.7494	–1.3741
Bi(1)	0.0000	0.0000	2.0012
Bi(2)	0.0000	0.0000	–2.0012

[a] All coordinates in Å.

Energy = –1894.96409 Hartrees (corrected for ZPE)

Table S22 Calculated [BLYP/aug-cc-pVTZ-PP/6-311G*] coordinates for $Bi_2(C_6F_4)_3$.[a]

Atom	*x*	*y*	*z*
C(1)	0.0000	4.3476	0.7006
C(2)	0.0000	3.1205	1.3799
C(3)	0.0000	1.9026	0.7035
C(4)	0.0000	1.9026	–0.7035
C(5)	0.0000	3.1205	–1.3799
C(6)	0.0000	4.3476	–0.7006
F(7)	0.0000	5.5203	1.3745
F(8)	0.0000	3.1549	2.7535
F(9)	0.0000	3.1549	–2.7535
F(10)	0.0000	5.5203	–1.3745
C(1)′	–3.7652	–2.1738	0.7006
C(2)′	–2.7024	–1.5602	1.3799
C(3)′	–1.6477	–0.9513	0.7035
C(4)′	–1.6477	–0.9513	–0.7035
C(5)′	–2.7024	–1.5602	–1.3799
C(6)′	–3.7652	–2.1738	–0.7006
F(7)′	–4.7808	–2.7602	1.3745
F(8)′	–2.7323	–1.5775	2.7535
F(9)′	–2.7323	–1.5775	–2.7535
F(10)′	–4.7808	–2.7602	–1.3745
C(1)″	3.7652	–2.1738	0.7006
C(2)″	2.7024	–1.5602	1.3799
C(3)″	1.6477	–0.9513	0.7035
C(4)″	1.6477	–0.9513	–0.7035
C(5)″	2.7024	–1.5602	–1.3799
C(6)″	3.7652	–2.1738	–0.7006
F(7)″	4.7808	–2.7602	1.3745
F(8)″	2.7323	–1.5775	2.7535
F(9)″	2.7323	–1.5775	–2.7535
F(10)″	4.7808	–2.7602	–1.3745
Bi(1)	0.0000	0.0000	2.0242
Bi(2)	0.0000	0.0000	–2.0242

[a] All coordinates in Å.

Energy = –2313.34741 Hartrees (corrected for ZPE)