

Table 9. Torsion angles [$^{\circ}$] for C₄₂H₂₄ (LT).

C6	C1	C2	C3	14.6(3)	C3	C19	C20	C21	-173.2(2)
C7	C1	C2	C3	-156.1(2)	C19	C20	C21	C22	0.6(3)
C6	C1	C2	C18	-156.6(2)	C20	C21	C22	C23	0.7(3)
C7	C1	C2	C18	32.7(2)	C21	C22	C23	C24	-1.3(3)
C1	C2	C3	C4	-15.3(3)	C20	C19	C24	C23	0.7(3)
C18	C2	C3	C4	155.3(2)	C3	C19	C24	C23	172.7(2)
C1	C2	C3	C19	157.0(2)	C20	C19	C24	C25	-178.3(2)
C18	C2	C3	C19	-32.4(3)	C3	C19	C24	C25	-6.3(3)
C2	C3	C4	C5	16.6(3)	C22	C23	C24	C19	0.6(3)
C19	C3	C4	C5	-156.2(2)	C22	C23	C24	C25	179.5(2)
C2	C3	C4	C30	-153.9(2)	C19	C24	C25	C26	-158.6(2)
C19	C3	C4	C30	33.2(2)	C23	C24	C25	C26	22.5(3)
C3	C4	C5	C6	-17.7(3)	C19	C24	C25	C30	19.3(3)
C30	C4	C5	C6	152.5(2)	C23	C24	C25	C30	-159.6(2)
C3	C4	C5	C31	153.5(2)	C30	C25	C26	C27	-1.4(3)
C30	C4	C5	C31	-36.4(3)	C24	C25	C26	C27	176.5(2)
C4	C5	C6	C1	16.9(3)	C25	C26	C27	C28	0.4(3)
C31	C5	C6	C1	-154.7(2)	C26	C27	C28	C29	-0.3(3)
C4	C5	C6	C42	-154.7(2)	C27	C28	C29	C30	1.2(3)
C31	C5	C6	C42	33.7(2)	C28	C29	C30	C25	-2.2(3)
C2	C1	C6	C5	-15.6(3)	C28	C29	C30	C4	-171.5(2)
C7	C1	C6	C5	154.5(2)	C26	C25	C30	C29	2.3(3)
C2	C1	C6	C42	155.4(2)	C24	C25	C30	C29	-175.7(2)
C7	C1	C6	C42	-34.5(3)	C26	C25	C30	C4	171.8(2)
C2	C1	C7	C12	-20.4(2)	C24	C25	C30	C4	-6.2(3)
C6	C1	C7	C12	169.3(2)	C3	C4	C30	C29	148.7(2)
C2	C1	C7	C8	150.0(2)	C5	C4	C30	C29	-21.6(3)
C6	C1	C7	C8	-20.3(3)	C3	C4	C30	C25	-20.5(3)
C12	C7	C8	C9	-1.9(3)	C5	C4	C30	C25	169.2(2)
C1	C7	C8	C9	-172.5(2)	C6	C5	C31	C32	148.6(2)
C7	C8	C9	C10	-0.6(3)	C4	C5	C31	C32	-22.7(3)
C8	C9	C10	C11	2.1(3)	C6	C5	C31	C36	-22.0(3)
C9	C10	C11	C12	-0.9(3)	C4	C5	C31	C36	166.7(2)
C8	C7	C12	C11	3.0(3)	C36	C31	C32	C33	-3.0(3)
C1	C7	C12	C11	173.7(2)	C5	C31	C32	C33	-173.7(2)
C8	C7	C12	C13	-175.3(2)	C31	C32	C33	C34	0.2(3)
C1	C7	C12	C13	-4.6(3)	C32	C33	C34	C35	1.7(3)
C10	C11	C12	C7	-1.6(3)	C33	C34	C35	C36	-0.8(3)
C10	C11	C12	C13	176.6(2)	C34	C35	C36	C31	-1.9(3)
C7	C12	C13	C18	16.4(3)	C34	C35	C36	C37	176.8(2)
C11	C12	C13	C18	-161.9(2)	C32	C31	C36	C35	3.7(3)
C7	C12	C13	C14	-161.2(2)	C5	C31	C36	C35	174.6(2)
C11	C12	C13	C14	20.5(3)	C32	C31	C36	C37	-175.0(2)
C18	C13	C14	C15	-0.5(3)	C5	C31	C36	C37	-4.2(3)
C12	C13	C14	C15	177.1(2)	C35	C36	C37	C38	19.0(3)
C13	C14	C15	C16	-2.1(3)	C31	C36	C37	C38	-162.3(2)
C14	C15	C16	C17	2.0(3)	C35	C36	C37	C42	-161.0(2)
C15	C16	C17	C18	0.8(3)	C31	C36	C37	C42	17.7(3)
C14	C13	C18	C17	3.2(3)	C42	C37	C38	C39	-0.8(3)
C12	C13	C18	C17	-174.5(2)	C36	C37	C38	C39	179.2(2)
C14	C13	C18	C2	174.2(2)	C37	C38	C39	C40	-1.2(3)
C12	C13	C18	C2	-3.5(3)	C38	C39	C40	C41	1.3(3)
C16	C17	C18	C13	-3.4(3)	C39	C40	C41	C42	0.7(3)
C16	C17	C18	C2	-174.3(2)	C40	C41	C42	C37	-2.6(3)
C1	C2	C18	C13	-21.5(2)	C40	C41	C42	C6	-174.3(2)
C3	C2	C18	C13	167.7(2)	C38	C37	C42	C41	2.7(3)
C1	C2	C18	C17	149.3(2)	C36	C37	C42	C41	-177.3(2)
C3	C2	C18	C17	-21.5(3)	C38	C37	C42	C6	174.4(2)
C4	C3	C19	C24	-20.3(3)	C36	C37	C42	C6	-5.6(3)
C2	C3	C19	C24	167.2(2)	C5	C6	C42	C41	151.0(2)
C4	C3	C19	C20	151.5(2)	C1	C6	C42	C41	-20.2(3)
C2	C3	C19	C20	-21.0(3)	C5	C6	C42	C37	-20.5(3)
C24	C19	C20	C21	-1.3(3)	C1	C6	C42	C37	168.3(2)

Figures

1. Molecular structure of hexabenzotriphenylene drawn with 50% probability thermal ellipsoids for carbon atoms and spheres of arbitrary size for hydrogen atoms.
2. Molecular structure drawn with 50% probability thermal ellipsoids for all atoms.
3. "Side" view of the molecular structure (nonhydrogen atoms only) drawn with with 50% probability thermal ellipsoids.

Space-filling, ball-and-stick, and cell plots have not been included, since they are essentially indistinguishable from those in the room temperature structure report (RAP002).





