II.A.3. (XII.A.1.)

Listing of experimental geometry data for $CH_3CH_2CH_2CH_3$ (Butane)

Rotational Constants (cm^{-1})
See section I.F.4 to change rotational constant units

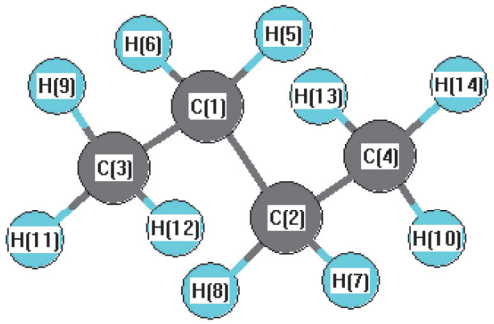
A	B	C

Rotational Constants from
Calculated rotational constants for $CH_3CH_2CH_2CH_3$ (Butane).

Point Group C_{2h}

Internal coordinates (distances (r) in Å) (angles (a) in degrees) (dihedrals (d) in degrees)

Description	Value	Connectivity				Reference	Comment
		Atom 1	Atom 2	Atom 3	Atom 4		
rCC	1.531	1	2			1998Kuc	rg
rCH	1.117	1	5			1998Kuc	rg
aCCC	113.8	2	1	3		1998Kuc	
aHCC	111	1	2	7		1998Kuc	average
d	64.9	3	1	2	4	1998Kuc	gauche



Bond descriptions
Examples: C-C single bond, C=C, double bond, C#C triple bond, C:C aromatic bond

Bond Type	Count
H-C	10
C-C	3

Atom	x (Å)	y (Å)	z (Å)

Atom - Atom Distances (Å)

Calculated geometries for $CH_3CH_2CH_2CH_3$ (Butane).

References

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squib	reference	DOI
1998Kuc	K Kuchitsu(ed) "Structure of Free Polyatomic Molecules - Basic Data" Springer, Berlin, 1998	

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