

Electronic supplementary information

**VIBRATIONAL SPECTRUM AND ELECTRONIC STRUCTURE OF
11-VERTEX *NIDO*-TRICARBABORANE 7,8,9- $C_3B_8H_{12}$
AS COMPARED TO ISOSTRUCTURAL $[7,9-C_2B_9H_{12}]^-$ SPECIES**

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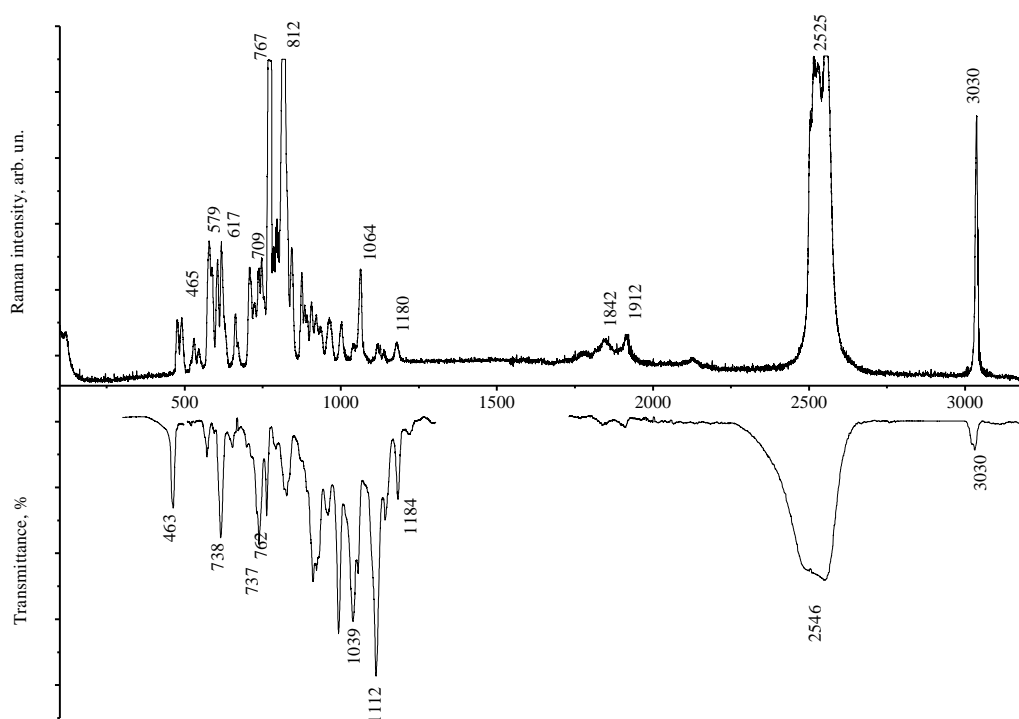
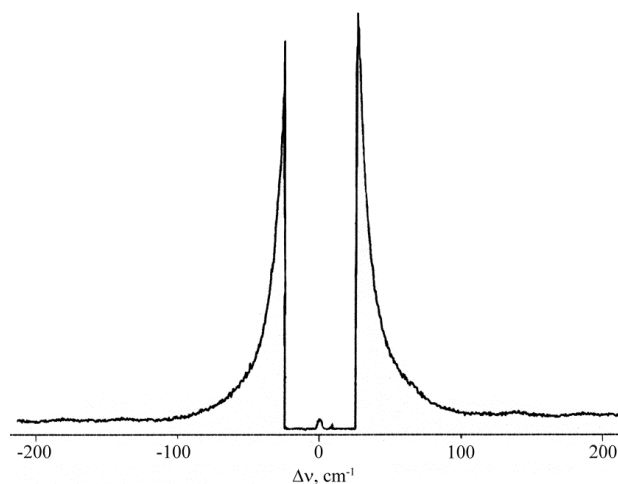
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ul. Vavilova 28, Moscow, 119991 Russia***Figure S1.** Raman and IR spectra of solid Cs [7,9-C₂B₉H₁₂]**Figure S2.** Broad Rayleigh wing in the low-frequency Raman spectrum of solid 7,8,9-C₃B₈H₁₂ (1)

Table S1. Vibrational spectrum of solid 7,8,9-tricarba-*nido*-undecaborane C₃B₈H₁₂

Calc.		Symmetry species	Experimental data		Assignment
ν , cm ⁻¹	IR intensity		IR	Raman (μ -d) ^a	
3204	0.6	A'			
3198	0	A''	3068 w	3070 s (3070)	vCH
3193	0.2	A'			
2714	95	A'		2624 (2620)	
2705	78	A''			
2695	94	A'		2597 (2595)	
2691	100	A''	2592 vs		vBH _t
2681	36	A'			
2673	112	A'			
2667	45	A'			
2662	42	A''			
				~2108w br	overtone
1989	3	A'		~1900m (1430)	v/ δ BHB
1715	0	A''	1790-2200	~1780vw (1380)	v/ δ BHB
1329	0.2	A''	1296 m	1297 w (1298)	δ CH
1290	4	A'	1252 ms	1255 w (1250)	δ CH
1199	16	A''	1164 s	1165 w (1152)	δ CH + δ BH
1137	10	A'	1116 ms	1115 w	δ CH + δ BH + H _b
1087	9	A'	1064 s	1065 w	δ CH + δ BH + H _b
1072	18	A''	1048 s	1050 w	δ BH + δ CH
1053	2	A'		1030 w	H _b + δ CH + δ BH
1052	0	A''	1024 w		δ CH + δ BH
1032	2	A'	1004 w	1008 wm	δ CH + H _b + δ BH
1012	5	A''	988 w		δ BH + δ CH
988	7	A'	968 s	966 w	δ BH + δ CH
982	0.7	A''			δ BH + δ CH + cage
961	1	A'			δ BH + δ CH + cage
955	0,0	A''			δ BH + cage
947	9,5	A'	944 w	944 w	δ BH + δ CH + cage
939	1	A''			δ BH + cage
935	2	A''			
935	8	A'		931w	δ BH + δ CH + cage
922	0,7	A''	928 m	922 sh	
917	1	A'	916 m		vCC+vCB+ δ CH+ δ BH
908	0,2	A''	904 w	903 m	δ BH + cage
899	22	A'	884 vs	886 w	δ CH+ δ BH+ H _b + cage
875	7	A'	860 s	860 ms	
848	0	A''			δ BH + cage
841	1	A'		835 w	
816	4	A'	828 w	826 m	δ BH + cage+ H _b
797	2	A'	804 w	806 vvs (797)	
792	0,2	A''	792 m	791 vs (774)	cage breathing
772	0.3	A'	772 w	769 s	δ BH + cage + H _b
772	0	A''			δ CH + cage
761	4	A''	752 m		cage + δ BH
744	1,5	A'			
736	2	A'		734 sh	cage + δ BH
736	7	A''	728 s		
725	3	A'		724 s	
709	0	A''			cage
694	0	A'	696 sh	694 m	
658	3	A'	656 ms	654 m	δ BH + cage
632	2	A'	640 ms	635 sh	vBB + H _b + cage + δ BH
620	0.2	A'		623 m	cage +H _b + δ BH

614	0	A''			cage.+ δ BH
590	0	A''			δ BH + cage
588	3	A'	584 m	585 m	
566	1	A'	572 sh	571 w	cage + H _b
551	5	A'	560 vs	558 sh	cage + H _b + δ CH
541	1	A''		549 w	cage deformation
515	0,4	A'		517 w	cage + δ BH
515	2	A''	516 s		cage + δ BH + H _b
494	0	A''		498 w (498)	cage + δ BH

^a μ -d – frequencies of similar vibrations in the Raman spectrum of deuterated molecule C₃B₈H₁₁D

Table S2. Vibrational spectra of solid Cs [7,9-C₂B₉H₁₂]⁻ and its μ -*d*-analog

Calc.		Symmetry species	Experimental data		Assignment
ν , cm ⁻¹	IR intensity		IR	Raman (μ - <i>d</i>) ^a	
3187	19	A'			
3186	35	A''	3030 m	3032s (3032)	ν CH
2665	200	A'			
2648	446	A''	2560 vs br	2550vs (2550)	
2643	441	A'			
2637	55	A'			
2635	7	A''		2525sh (2525)	ν BH _t
2629	90	A'		2515vs (2512)	
2598	105	A''		2502sh (2502)	
2696	227	A'			
1991	30	A'	1910w	1915w br (1445)	ν/δ BHB
1697	8	A''	1775w	1815w (1380)	ν/δ BHB
1201	3	A'	1183m	1182w (1181)	δ CH
1152	7	A''	1143sh		δ CH
1140	74	A''		1138w br	δ CH + δ BH
1133	0	A'		1126vw	
1103	10	A'	1112s	1115w br (1057)	H _b + δ CH + δ BH
1071	2	A''	1059sh	1060m (1045)	δ CH
1052	37	A'	1042m	1038w br (1000)	δ CH + δ BH + H _b
1008	2	A''		1000 w br	δ BH
993	27	A'	996m		δ CH + δ BH
974	1	A''			
963	10	A'	960m	961w br	δ BH + H _b
960	0	A''			
947	8	A'			
939	0	A''		932w (930)	
938	21	A'	927m		δ BH + cage
923	0	A''			
920	3	A'	915m	919w (911)	
915	1	A''			
903	1	A'	890m	905m	δ BH + δ CH + cage.
894	0	A''		890 sh	δ BH + δ CH + cage.
886	0,2	A''		883 sh	δ CH + δ BH + cage
876	2	A'		873m (871)	cage + δ BH
844	1	A'		841m (831)	δ BH + cage +
825	3	A'	830m		cage + δ BH + H _b
809	1	A''	825m		
805	0	A'		812vvs (811)	cage + δ BH + δ CH
797	0	A'	790w	794 m	
783	0	A''			cage + δ BH
782	0	A''		783 w	δ BH + cage
768	2	A'		767vs (772)	cage
764	2	A''	760 m		cage deform.
741	3	A'		739sh (746)	cage + δ BH
740	4	A''	735m		
731	3	A'	720sh	728m (730)	cage deform.
714	1	A''		715sh (713)	
710	0	A'	695sh	699s (700)	cage + δ BH
694	0	A'		662sh	
646	2	A'	652w	653w	
608	7	A'	618s	608 m	
607	1	A'	594 w	596s (596)	cage
602	0	A''			
587	0	A'		577m (575)	

576	0	A''	573m		
566	3	A'		545w	
558	1	A''	533vw	536 w	
527	0	A'			
508	1	A''	510w		
501	0	A''			cage deform.
464	0	A''		478 m (478)	
460	7	A'	463 m	462m (462)	

^a μ -d – frequencies of similar vibrations in the Raman spectrum of deuterated molecule C₂B₉H₁₁D