Electronic Supplementary Information

A facile synthesis for $BeCl_2$, $BeBr_2$ and BeI_2

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Powder X-ray diffraction

Powder X-ray diffraction was performed with a STOE StadiMP powder diffractometer using Cu-K α_1 radiation, a Ge monochromator and a Mythen1K detector. Samples were prepared under glovebox atmosphere in Lindemann capillaries of fused silica, which were flame sealed.

RIETVELD refinement

Phase analysis was performed with WinXPOW,¹ profiles were fitted with JANA2006.² RIETVELD refinement was carried out with JANA2006 using single crystal data from the literature.^{3–5}

IR spectroscopy

The IR spectra were recorded on a BRUKER Alpha II spectrometer with diamond ATR module inside an argon filled glovebox. Processing of the spectra was performed with the OPUS⁶ software package and OriginPro8.⁷

Raman spectroscopy

For the Raman spectroscopic measurements a small amount of the respective beryllium halide was collected and flames sealed in boro silicate capillaries with an inner diameter of 0.5 mm. Raman spectra were recorded on a RENISHAW inVia Qontor spectrometer at laser wavelengths of 457 nm, 532 nm, 633 nm and 785 nm and on a RENISHAW inVia Raman microscope at a laser wavelength of 785 nm

DFT calculations

All DFT calculations were carried out with the CRYSTAL14 program package using the PBE+D2 method. The *k*-mesh sampling was 8 x 8 for all studied compounds and the convergence criterion was set to 10^{-8} Hartree. The applied Basis sets were taken from $^{8-11}$. For the evaluation of the Coulomb and Exchange integrals (TOLINTEG), tolerance factors of 8 8 8 8 and 16 were used. After all full structural optimization including all lattice and atomic site parameters, the IR and Raman active vibrational modes including intensities were calculated. No imaginary frequencies were obtained.



Fig. 1 X-ray powder diffractograms with LeBail profile fit, difference plot and related reference for a) BeCl₂^{3,4}, b) BeBr₂⁵ and c) Bel₂⁵.



Fig. 2 $BeCl_2$ prior to fractionated sublimation.



Fig. 3 Unknown lint in the lower part of the ampoule in which ${\rm BeCl}_2$ was synthesised.



Fig. 4 $BeBr_2$ crystals after sublimation.



Fig. 5 Crystals of Bel_2 at the flame sealed end of the reaction ampule.

Еx	perimental	and	calculated	IR	and	Raman	data	for	BeF ₂	, BeCl ₂	, BeBr	and	Bel	2.
	Ex	Experimental	Experimental and	Experimental and calculated	Experimental and calculated IR	Experimental and calculated IR and	Experimental and calculated IR and Raman	Experimental and calculated IR and Raman data	Experimental and calculated IR and Raman data for	Experimental and calculated IR and Raman data for BeF ₂	Experimental and calculated IR and Raman data for BeF ₂ , BeCl ₂	Experimental and calculated IR and Raman data for BeF ₂ , BeCl ₂ , BeBr ₂	Experimental and calculated IR and Raman data for BeF ₂ , BeCl ₂ , BeBr ₂ and	Experimental and calculated IR and Raman data for BeF ₂ , BeCl ₂ , BeBr ₂ and Bel

$\alpha - \beta - BeF_2$		$\alpha - \beta - BeCl$	2	α -BeBr ₂		β -BeI ₂	
		IR d	ata / cm ⁻¹ ; experiment (ca	alculated) [mo	de]	, 2	
403	(β: 380) [E ₁]	450	$(\alpha: 449) [B_{1u}]$	404	$(400) [B_{1u}]$	450	$(462)[E_u]$
	(α: 388) [E]		$(\beta: 451) [A_{2u}]$	416		516	
	(β: 393) [A ₂]		$(\beta: 462) [E_u]$	462	(492) [B _{2u}]	581	
	(α: 412) [A ₂]	583	$(\alpha:560) [B_{3u}]$	477	(505) [B _{3u}]		
734	(α: 745) [A ₂]		(β: 563) [Eu]				
	(α: 747) [E]		(β: 563) [Eu]				
	(β: 754) [E ₁]		(β: 569) [A _{2u}]				
	(β: 756) [A ₂]		$(\alpha: 572) [B_{2u}]$				
		Rama	n data / cm $^{-1}$; experiment	(calculated) [r	node]		
		174	$(\alpha: 169) [B_{3g}]$	94	(99) [A _g]	76	(66) $[A_{1g}]$
			$(\alpha: 175) [B_{2g}]$	112	$(111) [B_{2g}]$		(68) $[B_{1g}]$
		290	$(\beta: 292) [A_{1g}]$		$(114) [B_{3g}]$		(72) $[E_g]$
		337	(α: 334) [Ag]	168	$(175) [B_{1g}]$		(74) $[B_{2g}]$
		410	$(\alpha: 385) [B_{3g}]$	203	(203) $[A_g]$		(76) $[A_{1g}]$
		416	$(\alpha: 388) [B_{2g}]$	374	(362) $[B_{3g}]$	92	(85) $[E_g]$
				585	(606) $[B_{1g}]$		(88) $[B_{2g}]$
							(92) $[E_g]$
						109	(102) [Eg]
							$(103) [B_{1g}]$
							$(109) [B_{2g}]$
							$(111) [E_g]$
							$(112) [E_g]$
						101	$(118) [A_{1g}]$
						131	$(132) [B_{1g}]$
							$(130) [E_g]$
						140	$(143) [A_{1g}]$
						140	$(147) [E_g]$
						260	$(146) [D_{2g}]$
						300	$(350) [D_{2g}]$
						420	$(331) [E_g]$
						430	$(410) [E_g]$
						4473	$(441) [D_{2g}]$ (485) [Δ]
						7/5	$(486) [B_{-}]$
							(401) [B,]
							$(\forall j \downarrow j \downarrow J \downarrow D]_{g}$

Table 2 Calculated IR and Raman vibrational modes for ${\rm BeF}_2.$

α –BeF ₂ , IR active modes		
wavenumber / cm ⁻¹	irreducible representation	intensity / km mol ⁻¹
90	E	0
187	E	0
280	A ₂	16
302	E	3
388	E	303
412	A ₂	181
596	E	3
745	A ₂	1354
747	E	2645
793	E	3
831	A ₂	6
866	Ē	53
α -BeF. Baman active modes		
wavenumber / cm^{-1}	irreducible representation	intensity / a 11
90	F	01
130	Δ.	262
197	A] E	202 A7
302	E	72
302	Δ.	1000
317		621
388	A] E	172
506	E	62
746	Δ.	02
740	A] E	33 49
747	E	42 2
795 866	E	5 21
	L	51
β -BeF ₂ , IR active modes		
wavenumber / cm ⁻¹	irreducible representation	intensity / km mol ⁻¹
66	E1	0
380	E_1	321
393	A ₂	228
754	E_1	2714
756	A ₂	1352
792	E ₁	0
β –BeF ₂ , Raman active modes		
wavenumber / cm ⁻¹	irreducible representation	intensity / a.u.
66	E1	58
180	E ₂	30
295	E ₂	16
316	A ₁	1000
380	E1	101
602	E ₂	58
754	E ₁	14
792	E ₁	3
875	E ₂	6

Table 3 Calculated IR and Raman vibrational modes for α -BeCl	2.
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α -BeCl ₂ , IR active modes		
wavenumber / cm ⁻¹	irreducible representation	intensity / km mol ⁻¹
170	B_{2u}	0
170	B_{3u}	0
449	B_{1u}	1228
560	B_{3u}	402
572	B_{2u}	385
α -BeCl ₂ , Raman active modes		
wavenumber / cm ⁻¹	irreducible representation	intensity / a.u.
62	B _{1g}	0
150	Ag	276
169	B_{3g}	189
175	B_{2g}	201
293	B_{1g}	355
334	Ag	1000
385	B_{3g}	71
388	B_{2g}	60
684	B_{1g}	38

Table 4 Calculated IR and Raman vibrational modes for β -BeCl₂.

	p – BeCl ₂ , IR active modes		
	wavenumber / cm ⁻¹	irreducible representation	intensity / km mol ^{-1}
_	57	Ē	0
	83	F	0
	00 00	E	
	100	E _u	
	108	Eu	1
	129	A_{2u}	2
	138	A_{2u}	0
	153	E_{μ}	6
	176	A	27
	170	F	13
	107		E
	197	E_u	5
	215	E_u	21
	226	E_u	12
	227	A_{2u}	14
	232	Eu	2
	296	 Е.,	1
	328	<u>–</u> u F	16
	220	Δ	10
	329	A_{2u}	2
	429	E_u	32
	434	E_u	5
	451	A_{2u}	5577
	462	Eu	7503
	556	A2	2
	563	F	
	505		2732
	503	E_u	1/42
	569	A_{2u}	825
	588	Eu	60
-	B-BeCla Raman active modes		
_	p been, reaman active modes	innederalle annual i si	intensity / a st
_	wavenumber / cm ⁻¹	irreducible representation	intensity / a.u.
	36	B_{2g}	4
	41	E	0
	46	Ĕ	14
		۸ ⁸	10
	80	A1	10
	80 81	R _{1g}	2
	80 81	Alg Eg	2
	80 81 88	$ \begin{array}{c} A_{1g} \\ E_{g} \\ E_{g} \\ E_{g} \end{array} $	2 5 5
	80 81 88 89	$\begin{array}{c} A_{1g} \\ E_{g} \\ E_{g} \\ B_{1g} \end{array}$	2 5 6
	80 81 88 89 109	$\begin{array}{c} \Lambda_{1g} \\ E_g \\ E_g \\ B_{1g} \\ E_g \end{array}$	2 5 6 6
	80 81 88 89 109 123	$ \begin{array}{c} \Lambda_{1g} \\ E_g \\ B_{1g} \\ E_g \\ B_{2g} \end{array} $	2 5 6 6 0
	80 81 88 89 109 123 137	$ \begin{array}{c} \Lambda_{1g} \\ E_{g} \\ E_{g} \\ B_{1g} \\ E_{g} \\ B_{2g} \\ A_{1g} \end{array} $	2 5 6 6 0 99
	80 81 88 89 109 123 137 130	$\begin{array}{c} A_{1g} \\ E_g \\ E_g \\ B_{1g} \\ E_g \\ B_{2g} \\ A_{1g} \\ B_g \end{array}$	2 5 6 6 0 99
	80 81 88 89 109 123 137 139 142	$\begin{array}{c} \Lambda_{1g} \\ E_g \\ E_g \\ B_{1g} \\ E_g \\ B_{2g} \\ \Lambda_{1g} \\ B_{1g} \end{array}$	2 5 6 6 0 99 97
	80 81 88 89 109 123 137 139 142	$\begin{array}{c} A_{1g} \\ E_g \\ E_g \\ B_{1g} \\ E_g \\ B_{2g} \\ A_{1g} \\ B_{1g} \\ B_{2g} \end{array}$	2 5 6 6 0 99 97 10
	80 81 88 89 109 123 137 139 142 146	$\begin{array}{c} A_{1g} \\ E_g \\ E_g \\ B_{1g} \\ E_g \\ B_{2g} \\ A_{1g} \\ B_{1g} \\ B_{2g} \\ A_{1g} \end{array}$	2 5 6 6 99 97 10 52
	80 81 88 89 109 123 137 139 142 146 150	$\begin{array}{c} A_{1g} \\ E_g \\ E_g \\ B_{1g} \\ E_g \\ B_{2g} \\ A_{1g} \\ B_{1g} \\ B_{2g} \\ A_{1g} \\ B_{2g} \\ A_{1g} \\ E_g \end{array}$	2 5 6 6 9 9 9 7 10 52 118
	80 81 88 89 109 123 137 139 142 146 150 175	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} B_{2g} A_{1g} B_{2g} B_{2g} A_{1g} B_{2g} B_{2g} A_{2g} B_{2g}	2 5 6 6 9 99 97 97 10 52 118 0
	80 81 88 89 109 123 137 139 142 146 150 175 179	$\begin{array}{c} A_{1g} \\ E_g \\ E_g \\ B_{1g} \\ E_g \\ B_{2g} \\ A_{1g} \\ B_{1g} \\ B_{2g} \\ A_{1g} \\ E_g \\ B_{1g} \\ E_g \\ B_{1g} \\ E_g \\ B_{1g} \\ E_g \\ B_{1g} \\ E_g \end{array}$	2 5 6 6 9 99 97 10 52 118 0 58
	80 81 88 89 109 123 137 139 142 146 150 175 179 180	$\begin{array}{c} A_{1g} \\ E_g \\ E_g \\ B_{1g} \\ E_g \\ B_{2g} \\ A_{1g} \\ B_{1g} \\ B_{2g} \\ A_{1g} \\ B_{2g} \\ A_{1g} \\ E_g \\ B_{1g} \\ E_g \\ B_{1g} \\ E_g \\ B_{2g} \end{array}$	2 5 6 6 9 9 9 9 7 10 52 118 0 58 206
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199	A_{1g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{1g} B_{2g} A_{1g} B_{1g} B_{2g} A_{1g} B_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{2g} A_{2g} A_{2g} B_{2g} A_{2g} B_{2g} A_{2g} B_{2g} A_{2g} B_{2g} A_{2g} B_{2g} A_{2g} B_{2g} A_{2g} B_{2g} A_{2g} B_{2g} A_{2g} B_{2g} A_{2g} B_{2g} A_{2g} B_{2g}	2 5 6 6 9 99 97 10 52 118 0 58 206 2
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} B_{2g} A_{1g} E_{g} B_{2g} $B_{$	2 5 6 6 9 99 97 10 52 118 0 58 206 2
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{1g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} A_{2g} A_{2g} A_{2g} B_{2g} A_{2g} B_{2g} B_{2g} A_{2g} B_{2g} B_{2g} A_{2g} B_{2	2 5 6 6 9 99 97 77 10 52 118 0 58 206 2 152
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{1g} E_{g} B_{2g}	2 5 6 6 9 9 9 9 7 10 52 118 0 58 206 2 2 152 29
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226	A_{1g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g}	2 5 6 6 9 9 99 97 10 52 118 0 58 206 2 152 29 10
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} B_{2g} A_{1g} E_{g} B_{2g} B_{2g} E_{g} B_{2g}	2 5 6 6 9 9 99 97 10 52 118 0 58 206 2 152 29 10 0
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{1g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} $E_{$	2 5 6 6 9 9 99 97 10 52 118 0 58 206 2 152 29 10 0 7
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g}	2 5 6 6 9 9 9 9 7 10 52 118 0 58 206 2 2 152 29 10 0 7 8 5
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 201	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{2g} A_{1g} E_{g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g}	2 5 6 6 9 9 9 9 9 7 10 52 118 0 58 206 2 152 29 10 0 7 85
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} B_{2g} E_{g} B_{2g}	2 5 6 6 9 9 9 9 7 10 52 118 0 58 206 2 152 29 10 0 0 7 8 5 9 9
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{1g} A_{1g} B_{1g} A_{1g}	2 5 6 6 9 9 99 97 10 52 118 0 58 206 2 152 29 10 0 7 85 19 10 00
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{1g} B_{2g} A_{1g} B_{2g} B_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{2g	2 5 6 6 9 9 9 9 7 10 52 118 0 58 206 2 2 152 29 10 0 7 7 8 5 19 1000 4
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g}	2 5 6 6 9 9 9 9 9 7 10 52 118 0 58 206 2 2 152 29 10 0 7 8 5 8 5 19 10000 41 15
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330	A_{1g} E_g E_g B_{1g} E_g B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} E_g B_{1g} E_g B_{2g} E_g B_{2g} E_g B_{2g} E_g B_{2g} E_g B_{1g} B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g B_{2g} E_g B_{2g} E_g B_{2g} E_g B_{2g}	2 5 6 6 9 9 99 97 10 52 118 0 58 206 2 152 29 10 0 7 85 19 10 0 7 85 19
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} E_{g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} E_{g} B_{2g} E_{g} B_{1g} A_{1g} B_{2g} E_{g}	2 5 6 6 9 9 99 97 10 52 118 0 58 206 2 152 29 10 0 0 7 85 19 1000 41 15 8 1
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 432	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{1g} B_{2g} A_{1g} B_{2g} B_{2g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g}	2 5 6 6 9 9 9 9 7 10 52 118 0 58 206 2 2 152 29 10 0 7 8 5 19 1000 41 15 8 8 19
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g}	2 5 6 6 9 9 9 9 9 7 10 52 118 0 58 206 2 2 152 29 10 0 7 8 5 19 1000 41 15 8 8 19
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} E_{g} B_{2g} E_{g} E_{g} E_{g} B_{2g} E_{g}	2 5 6 6 99 99 97 10 52 118 0 58 206 2 152 29 10 0 7 85 19 1000 41 15 8 19
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 228 232 245 291 292 296 327 330 430 432 446 453	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} B_{2g} E_{g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} E_{g} B_{2g} E_{g} E_{g} E_{g} B_{2g} E_{g} E	2 5 6 6 9 9 9 9 7 10 52 118 0 58 206 2 152 29 10 0 7 8 5 19 1000 41 15 8 5 19
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446 453 462	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} B_{2g} E_{g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{1g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} E_{g} E_{g} E_{g} B_{1g} B_{2g} E_{g} $E_$	2 5 6 6 9 9 9 9 7 10 5 2 118 0 5 8 206 2 152 29 10 0 0 7 8 5 19 10 0 0 7 8 5 19 10 0 0 7 8 5 19 10 0 0 7 8 5 19 10 0 7 8 5 19 10 0 7 7 8 5 19 10 10 5 8 206 2 15 2 2 15 2 2 9 7 10 5 8 206 2 15 2 2 15 2 2 9 7 10 5 8 206 2 15 2 2 9 9 10 5 8 206 2 15 2 2 9 10 10 5 8 206 2 11 8 10 10 5 8 206 2 15 2 15 2 2 9 10 10 5 8 2 10 10 5 8 2 10 10 10 10 10 10 10 10 10 10 10 10 10
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446 453 462 555	A_{1g} E_g E_g B_{1g} E_g B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} B_{2g} E_g B_{1g} E_g B_{2g} E_g B_{2g} E_g B_{2g} E_g B_{2g} E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g E_g B_{2g} E_g E_g E_g E_g B_{2g} E_g	2 5 6 6 6 9 9 9 9 9 7 10 5 8 20 6 2 15 2 2 15 2 2 9 10 0 7 8 5 19 1000 41 15 8 8 1 9 1000 41 15 8 5 8 1 19 1000 7 7 8 5 8 5 8 5 8 5 7 7 7 7 7 7 7 7 7 7
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446 453 462 555 558	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} B_{2g} E_{g} B_{2g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} B_{2g} E_{g} B_{2g} $B_$	2 5 6 6 6 9 9 9 9 9 9 9 7 10 5 2 20 6 2 15 2 9 9 10 0 7 8 5 8 1 9 9 1000 4 1 15 8 8 1 9 9 9 7 3 5 8 6
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 228 232 245 291 292 296 327 330 430 432 446 453 462 555 558 559	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} E_{g} B_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} B_{2g} B_{2g} $B_$	2 5 6 6 6 9 9 9 9 9 7 10 0 5 8 118 0 5 8 20 6 2 152 29 10 0 0 7 8 5 19 1000 41 15 8 8 1 9 9 9 7 3 5 6 1
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446 453 462 555 558 559 550	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} B_{2g} E_{g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{1g} B_{2g} E_{g} E_{g} E_{g} E_{g} E_{g} B_{1g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{2g} E_{g} E_{g} B_{2g} B_{2g} B_{2g} B_{2g} B_{2g} B_{2g} B_{2g}	2 5 6 6 9 9 9 9 9 9 7 10 5 2 118 0 5 8 206 2 2 152 29 10 0 7 8 5 9 9 9 9 9 7 3 5 4
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446 453 462 555 558 559 560	A_{1g} E_g E_g B_{1g} E_g B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} B_{2g} E_g B_{1g} E_g B_{2g} E_g B_{2g} E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{1g} B_{2g} E_g E_g E_g E_g E_g B_{1g} B_{2g} E_g $E_$	2 5 6 6 9 9 9 9 9 7 10 5 2 118 0 5 8 206 2 2 152 29 10 0 7 8 5 19 10 0 7 8 5 19 1000 4 1 15 8 8 19 1000 7 8 5 8 5 9 9 7 3 5 5 8 19 10 10 5 2 2 11 10 5 2 2 11 12 2 9 10 10 5 2 2 15 2 2 9 10 10 5 2 2 15 2 2 9 10 10 5 2 2 15 2 2 9 10 10 5 2 2 15 2 2 9 10 10 5 8 2 15 2 2 9 10 10 5 8 2 15 2 2 9 10 10 5 8 5 10 10 5 8 2 15 2 2 9 10 10 5 7 8 5 19 10 10 5 8 5 19 10 10 5 7 8 5 19 10 10 10 10 10 10 10 10 10 10 10 10 10
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446 453 462 555 558 559 560 565	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{2g} A_{1g} E_{g} B_{1g} E_{g} B_{2g} E_{g} B_{2g} E_{g} B_{2g} B_{2g} E_{g} B_{2g}	2 5 6 6 9 9 9 9 9 9 7 10 5 2 118 0 5 2 206 2 152 29 10 0 0 7 8 5 19 1000 41 15 8 5 19 1000 41 15 8 5 19 1000 5 7 8 5 19 1000 5 7 8 5 19 1000 5 7 8 5 19 1000 5 7 8 5 19 1000 5 7 8 5 19 1000 5 7 8 5 19 1000 5 7 8 5 19 1000 5 7 8 5 19 1000 5 7 8 5 10 7 7 8 5 19 10 10 7 7 8 5 19 10 10 7 7 8 5 19 10 10 7 7 8 5 19 10 10 7 7 8 5 19 10 10 7 7 8 5 19 10 10 7 7 8 5 19 10 10 10 10 10 10 10 10 10 10 10 10 10
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 228 232 245 291 292 296 327 330 432 446 453 462 555 558 559 560 565 572	A_{1g} E_g E_g B_{1g} E_g B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} B_{2g} E_g B_{1g} E_g B_{2g} E_g E_g E_g E_g B_{1g} B_{2g} E_g	2 5 6 6 7 99 97 10 52 118 0 58 206 2 152 29 10 0 7 85 19 10 0 7 85 19 1000 41 15 8 8 1 1 9 1000 7 7 85 19 1000 7 7 85 19 10 1000 7 7 85 19 10 10 5 7 85 19 10 10 5 8 5 19 10 10 5 7 7 8 5 19 10 10 5 7 8 5 10 5 7 5 8 5 10 10 5 7 5 8 5 10 5 7 5 7 5 7 5 7 5 7 5 7 5 7 5 7 5 7 5
	80 81 88 89 109 123 137 139 142 146 150 177 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446 453 462 555 558 559 560 572 593	A_{1g} E_g E_g B_{1g} E_g B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} A_{1g} E_g B_{2g} E_g B_{2g} E_g	2 5 6 6 9 9 9 9 7 10 5 2 118 0 5 8 206 2 152 29 10 0 7 8 5 19 1000 41 15 8 8 19 1000 41 15 8 8 19 1000 41 15 8 8 15 2 9 9 7 3 5 5 8 10 10 10 5 7 10 10 10 10 10 10 10 10 10 10 10 10 10
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446 453 462 555 558 559 560 565 572 593 605	A_{1g} E_g E_g B_{1g} E_g B_{2g} A_{1g} B_{2g} A_{1g} B_{2g} B_{2g} E_g B_{1g} E_g B_{2g} E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g E_g B_{2g} E_g E_g E_g B_{2g} E_g E_g E_g B_{2g} E_g E_g E_g E_g E_g E_g B_{2g} E_g	2 5 6 6 7 99 97 10 52 118 0 58 206 2 29 10 0 7 85 19 100 0 7 85 19 100 101 152 29 100 0 7 85 19 100 101 153 85 19 100 101 103 103 104 115 152 152 152 152 152 153 154 155 155 155 155 155 155 155
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 226 228 232 245 291 292 296 327 330 430 432 446 453 462 555 558 559 560 565 572 593 605 605 605	A_{1g} E_g E_g B_{1g} E_g B_{2g} A_{1g} B_{2g} A_{1g} E_g B_{1g} E_g B_{1g} E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} E_g E_g B_{2g} B_{2g} E_g B_{2g} B_{2g} E_g B_{2g} B_{2g} E_g B_{2g} B_{2g} E_g B_{2g} B_{2g} E_g B_{2g} B_{2	2 5 6 6 9 99 97 10 52 118 0 58 206 2 152 29 10 0 7 85 19 1000 41 15 8 1 9 1000 41 15 8 1 9 1000 41 15 8 1 9 1000 41 15 8 1 1 1 8 1 1 1 5 8 1 1 1 1 1 1 1 1 1 1 1 1 1
	80 81 88 89 109 123 137 139 142 146 150 175 179 180 199 215 216 228 232 245 291 292 296 327 330 430 432 446 453 462 555 558 559 560 565 572 593 605 608 610	A_{1g} E_{g} E_{g} B_{1g} E_{g} B_{2g} A_{1g} B_{1g} B_{2g} A_{1g} B_{2g} B_{1g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} E_{g} B_{2g} E_{g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{1g} B_{2g} E_{g} B_{2g} B	2 5 6 6 9 99 97 10 52 118 0 58 206 2 152 29 10 0 7 85 19 1000 41 15 8 1 1000 41 15 8 8 1 1000 41 15 8 8 1 1000 41 15 8 8 1 1000 41 15 8 8 1 1 1 1 1 1 1 1 1 1 1 1 1

BeBr ₂ , IR active modes		
wavenumber / cm ⁻¹	irreducible representation	intensity / km mol ⁻¹
108	B _{2u}	0
109	B_{3u}	0
400	B_{1u}	1160
492	B_{2u}	349
505	B_{3u}	347
BeBr ₂ , Raman active modes		
wavenumber / cm ⁻¹	irreducible representation	intensity / a.u.
45	B _{1g}	0
99	Ag	336
111	B_{2g}	220
114	B_{3g}	239
175	B_{1g}	399
203	Ag	1000
358	B_{2g}	215
362	B _{3g}	220
606	B _{1g}	23

Table 5 Calculated IR and Raman vibrational modes for $\mbox{BeBr}_2.$

Table 6 Calculated IR and Raman vibrational modes for $\alpha-\text{Bel}_2.$

α –BeI ₂ , IR active modes		
wavenumber / cm^{-1}	irreducible representation	intensity / km mol $^{-1}$
83	B _{2u}	0
87	B_{3u}	0
365	B_{1u}	1181
435	B_{2u}	360
454	B _{3u}	351
α -BeI ₂ , Raman active modes		
wavenumber / cm^{-1}	irreducible representation	intensity / a.u.
51	B _{1g}	1
82	B_{2g}	263
87	A_g	433
88	B_{3g}	309
119	B_{1g}	497
147	Ag	1000
340	B_{2g}	241
343	B_{3g}	217
519	B _{1g}	20

Table 7 Calculated IR and Raman vibrational modes for β -Bel₂.

β -BeI ₂ , IR active modes		
wavenumber / cm ⁻¹	irreducible representation	intensity / km mol ⁻¹
41	E_u	0
47	E_u	0
53	E_u	0
58	E_u	0
68	A_{2u}	0
71	A_{2u}	0
78	E_u	0
83	A_{2u}	0
84	E_u	1
93	E_u	0
103	E_u	1
108	E_u	8
109	A_{2u}	6
113	E_u	0
136	E_u	1
148	A_{2u}	0
148	E_u	2
349	A_{2u}	3926
351	E_u	4080
372	E_u	271
376	E_u	28
427	E_u	842
451	A_{2u}	157
456	\mathbf{E}_{u}	204
462	E_u	4306
463	A _{2u}	1624
β –BeI ₂ , Raman active modes		
wavenumber / cm ⁻¹	irreducible representation	intensity / a.u.
29	E _a	0
37	\mathbf{B}_{2g}°	1
39	E_g	8
46	$\tilde{E_g}$	0
46	A _{1g}	42
53	E_g	8
56	E_g	12
58	B_{2g}	5
59	B_{1g}	7
66	A_{1g}	154
68	\mathbf{B}_{1g}	244
72	\mathbf{E}_{g}	275
74	B_{2g}	8
76	A_{1g}	93
85	B_{1g}	0
85	Eg	149
88	B_{2g}	428
93	E _g	5
102	E _g	334 57
103	B_{1g}	5/
109	\mathbf{B}_{2g}	19
111	Eg	1
112	Eg	13 05
120	n_{1g}	52 52
134	D _{1g} F	55 100
1/2	Lig A	100
173 1 <i>1</i> 7	Alg F	1000
148	Bo	54
350	B ₂ g	רד רדי רדי
350	B _{2g} F	176
372	Eg F	0
375	Eg	42
379		2 2
416	- - 1g	- 65
110	E_	
419	E _g B ₁₋	0
419 441	E_g B_{1g} B_{2g}	0 41
419 441 447	$ \begin{array}{c} \mathbf{E}_{g}\\ \mathbf{B}_{1g}\\ \mathbf{B}_{2g}\\ \mathbf{E}_{g}\\ \mathbf{E}_{g} \end{array} $	0 41 5
419 441 447 458		0 0 41 5 8
419 441 447 458 462	$ E_{g} \\ B_{1g} \\ B_{2g} \\ E_{g} \\ A_{1g} \\ B_{1g} $	0 41 5 8 28
419 441 447 458 462 471		0 41 5 8 28 4
419 441 447 458 462 471 485	$ \begin{array}{l} E_g \\ B_{1g} \\ B_{2g} \\ E_g \\ E_g \\ A_{1g} \\ B_{1g} \\ E_g \\ A_{1e} \end{array} $	0 41 5 8 28 4 87
419 441 447 458 462 471 485 486	$ E_g B_{1g} B_{2g} E_g A_{1g} B_{2g} E_g A_{1g} B_{2g} $	0 41 5 8 28 4 87 37

Table 8 Optimized and experimental ^{5,12,13} (in brackets) lattice parameters in Å and cell volumes in Å³.

compound	а	b	С	V per formula unit
α – BeF ₂	4.821 (4.7390(5))		5.294 (5.1875(8))	53.27 (50.45(3))
$\beta - \text{BeF}_2$	4.910 (4.8060(1))		5.407 (5.2404(1))	56.45 (52.41(0))
$\alpha - \text{BeCl}_2$	5.305 (5.285(3))	10.309 (9.807(3))	5.336 (5.227(3))	72.95 (67.7(2))
$\beta - \text{BeCl}_2$	10.883 (10.595(5))		18.457 (18.036(7))	68.31 (63(2))
BeBr ₂	5.621 (5.569(4))	10.662 (10.405(6))	5.601 (5.543(3))	83.91 (80.3(3))
$\alpha - \tilde{Bel}_2$	5.867 (6.025(3))	11.494 (11.316(4))	5.994 (6.035(3))	101.05 (102.9(3))
$\beta - \text{Bel}_2$	11.962 (12.190(6))		21.796 (21.325(8))	97.46 (99(3))
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