SUPPLEMENTARY INFORMATION

Table S1 Linear coefficients, c_i, in the expansion of the distortion vector, normalized to 1, at the two different points, R = 0.12 (amu)$^{1/2}$Å and in the minimum, $R = R_{JT}$, of $^2A_2$ electronic state in C_{2v} geometry; correlation of the low symmetry vibrations to the high symmetry one is given; contribution of the vibration to the calculated E_{JT} in cm^{-1}. The most important vibrations are given in bold.

Symmetry in D_{5h}	$c_i(R = 0.12(\text{amu})^{1/2}\text{Å})$	$c_i(R = R_{JT})$	$E_{JT}^i(\text{cm}^{-1})$
e_1'	0.0000	0.0004	0.0121
a_1'	0.0000	0.0026	1.0562
e_1'	0.0009	0.0021	0.6525
e_2'	**0.4377**	**0.6490**	**348.1601**
a_1'	0.0002	0.0041	5.2601
e_1'	0.0321	0.0138	9.4111
e_2'	**0.1658**	**0.1004**	**112.0479**
e_2'	**0.0479**	**0.1216**	**137.0990**
e_1'	0.0031	0.0009	2.7961
e_2'	**0.2682**	**0.0833**	**133.7086**
a_1'	0.0001	0.0004	0.0012
e_2'	0.0238	0.0098	34.2503
e_1'	0.0139	0.0118	28.1925
e_2'	0.0003	0.0004	1.1785
e_1'	0.0001	0.0000	0.3532
a_1'	0.0000	0.0000	0.0205

Table S2 Linear coefficients, c_i, in the expansion of the distortion vector, normalized to 1, at the two different points R = 0.12 (amu)$^{1/2}$Å and in the minimum, $R = R_{JT}$, of $^2B_1$ electronic state in C_{2v} geometry; correlation of the low symmetry vibrations to the high symmetry one is given; contribution of the vibration to the calculated E_{JT} in cm^{-1}. The most important vibrations are given in bold.

Symmetry in D_{5h}	$c_i(R = 0.12(\text{amu})^{1/2}\text{Å})$	$c_i(R = R_{JT})$	E_{JT}^i (cm^{-1})
e_1'	0.0001	0.0001	0.0022
a_1'	0.0002	0.0042	0.5694
e_1'	0.0010	0.0013	0.2580
e_2'	**0.4351**	**0.6566**	**353.1893**
a_1'	0.0026	0.0010	0.8582
e_1'	0.0004	0.0056	5.0943
e_2'	**0.1812**	**0.1044**	**112.6036**
e_2'	**0.0478**	**0.1253**	**147.8086**
e_1'	0.0077	0.0022	3.4302
e_2'	**0.2866**	**0.0826**	**137.5563**
a_1'	0.0000	0.0002	0.3907
e_2'	0.0293	0.0113	33.4184
e_1'	0.0078	0.0051	16.3986
e_2'	0.0003	0.0001	1.5068
e_1'	0.0000	0.0000	0.3847
a_1'	0.0000	0.0000	0.0306

Table S1 Linear coefficients, c_i, in the expansion of the distortion vector, normalized to 1, at the the minimum of ^2A_g electronic state in C_{2h} geometry; correlation of the low symmetry vibrations to the high symmetry one is given; contribution of the vibration to the calculated E_{JT} in cm^{-1}. The most important vibrations are given in bold.

Symmetry in D_{5d}	$c_i(R = R_{JT})$	E_{JT}^i (cm^{-1})
e_{1g}	0.0068	0.5592
a_{1g}	0.0060	0.7398
e_{2g}	**0.4344**	**104.1473**
e_{1g}	0.0010	0.6999
a_{1g}	0.0076	6.2749
e_{2g}	**0.3046**	**301.4329**
e_{2g}	**0.3874**	**366.4795**
e_{1g}	0.0042	5.9264
e_{2g}	**0.0545**	**310.8962**
a_{1g}	0.0000	0.0150
e_{2g}	0.0138	36.4412
e_{1g}	0.0030	8.6534
e_{2g}	0.0001	1.7116
e_{1g}	0.0000	0.2016
a_{1g}	0.0000	0.0220

Table S8 Linear coefficients, c_i, in the expansion of the distortion vector, normalized to 1, at the the minimum of ^2B_g electronic state in C_{2h} geometry; correlation of the low symmetry vibrations to the high symmetry one is given; contribution of the vibration to the calculated E_{JT} in cm^{-1}. The most important vibrations are given in bold.

Symmetry in D_{5d}	$c_i(R = R_{JT})$	E_{JT}^i (cm^{-1})
e_{1g}	0.0069	0.8263
a_{1g}	0.0039	0.6406
e_{2g}	**0.4371**	**101.1266**
e_{1g}	0.0079	6.4389
a_{1g}	0.0000	0.0046
e_{2g}	**0.3080**	**99.7964**
e_{2g}	**0.3871**	**361.1295**
e_{1g}	0.0022	2.9325
e_{2g}	**0.0555**	**313.8749**
a_{1g}	0.0000	0.0122
e_{2g}	0.0141	36.5881
e_{1g}	0.0476	20.4280
e_{2g}	0.0001	1.0927
e_{1g}	0.0000	0.1385
a_{1g}	0.0000	0.0699