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Density Functional Theory Study of the Multimode Jahn-Teller Problem in the Fullerene Anion

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SUPPLEMENTARY INFORMATION

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TABLE S4 Analysis of the multimode JT problem of C_{60}^- in C_{2h} conformation by the LS totally symmetric normal modes in the harmonic approximation, IDP analysis at HS point, and the origin of the LS normal modes relative to the HS normal modes.

Table S1: Analysis of the multimode JT problem of C_{60}^- in D_{5d} conformation by the LS totally symmetric modes in the harmonic approximation. Frequencies (ν_k) of the selected normal modes are in cm^{-1} as obtained from DFT calculations. The contributions of the normal mode to the JT distortion (c_k) and the energy stabilization (E_k) are given in %. The origin of the LS normal mode relative to the HS normal mode is given.

LS	$^2A_{2u}$ (D_{5d})			Origin of the Irrep
Irrep	ν_k	c_k	E_k	
a_{1g}	260	30.14	4.87	h_g #1
a_{1g}	419	40.71	17.09	h_g #2
a_{1g}	500	0.08	0.05	a_g #1
a_{1g}	708	13.03	15.63	h_g #3
a_{1g}	788	4.80	7.15	h_g #4
a_{1g}	1125	1.96	5.94	h_g #5
a_{1g}	1268	0.87	3.37	h_g #6
a_{1g}	1455	5.21	26.41	h_g #7
a_{1g}	1511	0.03	0.14	a_g #2
a_{1g}	1595	3.17	19.35	h_g #8

Table S2: Analysis of the multimode JT problem of C_{60}^- in D_{3d} conformation by the LS totally symmetric modes in the harmonic approximation. Frequencies (ν_k) of the selected normal modes are in cm^{-1} as obtained from DFT calculations. The contributions of the normal mode to the JT distortion (c_k) and the energy stabilization (E_k) are given in %. The origin of the LS normal mode relative to the HS normal mode is given.

LS	$^2A_{2u}$ (D_{3d})			**Origin of the Irrep**
Irrep	ν_k	c_k	E_k	
a_{1g}	264	36.68	6.47	h_g #1
a_{1g}	428	36.25	16.81	h_g #2
a_{1g}	477	0.46	0.26	g_g #1
a_{1g}	503	0.04	0.03	a_g #1
a_{1g}	571	0.00	0.00	g_g #2
a_{1g}	707	11.69	14.85	h_g #3
a_{1g}	744	0.02	0.02	g_g #3
a_{1g}	789	4.32	6.81	h_g #4
a_{1g}	1116	0.31	0.99	h_g #5, g_g #4
a_{1g}	1125	1.72	5.53	g_g #4, h_g #5
a_{1g}	1273	0.62	2.55	h_g #6
a_{1g}	1326	0.02	0.09	g_g #5
a_{1g}	1461	4.73	25.57	h_g #7
a_{1g}	1511	0.04	0.23	a_g #2
a_{1g}	1518	0.00	0.00	g_g #6
a_{1g}	1586	3.10	19.78	h_g #8

Table S3: Analysis of the multimode JT problem of C_{60}^- in D_{2h} conformation by the LS totally symmetric modes in the harmonic approximation. Frequencies (ν_k) of the selected normal modes are in cm^{-1} as obtained from DFT calculations. The contributions of the normal mode to the JT distortion (c_k) and the energy stabilization (E_k) are given in %. The origin of the LS normal mode relative to the HS normal mode is given.

LS		**$^2B_{1u}$ (D_{2h})**				**$^2B_{2u}$ (D_{2h})**				**$^2B_{3u}$ (D_{2h})**		
irrep	**ν_k**	**c_k**	**E_k**	**Origin**	**ν_k**	**c_k**	**E_k**	**Origin**	**ν_k**	**c_k**	**E_k**	**Origin**
a_g	260	18.36	2.99	h_g #1	261	17.47	2.82	h_g #1	261	12.32	1.98	h_g #1
a_g	263	12.16	2.03	h_g #1	262	13.45	2.18	h_g #1	263	18.29	2.99	h_g #1
a_g	423	20.43	8.84	h_g #2	423	29.57	12.53	h_g #2	426	39.30	16.84	h_g #2
a_g	432	19.75	8.85	h_g #2	433	9.69	4.30	h_g #2	430	0.77	0.34	h_g #2
a_g	482	0.22	0.12	g_g #1	482	0.00	0.00	g_g #1	482	0.04	0.02	g_g #1
a_g	502	0.01	0.01	a_g #1	501	0.02	0.01	a_g #1	502	0.00	0.00	a_g #1
a_g	572	0.01	0.01	g_g #2	572	0.01	0.01	g_g #2	572	0.00	0.00	g_g #2
a_g	706	3.84	4.62	h_g #3	706	5.08	5.99	h_g #3	706	11.30	13.37	h_g #3
a_g	707	9.24	11.14	h_g #3	708	8.22	9.79	h_g #3	707	1.62	1.92	h_g #3
a_g	753	0.01	0.01	g_g #3	753	0.01	0.02	g_g #3	753	0.01	0.02	g_g #3
a_g	788	5.03	7.51	h_g #4	787	5.02	7.39	h_g #4	788	4.96	7.29	h_g #4
a_g	791	0.00	0.00	h_g #4	790	0.17	0.25	h_g #4	790	0.00	0.00	h_g #4
a_g	1114	0.05	0.14	h_g #5, g_g #4	1113	0.09	0.26	h_g #5, g_g #4	1114	0.13	0.38	h_g #5
a_g	1124	2.01	6.11	g_g #4, h_g #5	1123	2.06	6.16	h_g #5	1124	1.96	5.84	h_g #5
a_g	1131	0.05	0.15	h_g #5, g_g #4	1131	0.01	0.03	g_g #4, h_g #5	1131	0.09	0.27	h_g #5, g_g #4
a_g	1271	0.56	2.17	h_g #6	1271	0.57	2.18	h_g #6	1271	0.59	2.24	h_g #6
a_g	1278	0.06	0.23	h_g #6	1277	0.06	0.22	h_g #6	1277	0.08	0.32	h_g #6
a_g	1332	0.02	0.07	g_g #5	1331	0.01	0.05	g_g #5	1331	0.01	0.04	g_g #5
a_g	1447	0.20	0.99	h_g #7	1446	0.27	1.32	h_g #7	1447	0.26	1.30	h_g #7
a_g	1460	4.69	24.06	h_g #7	1460	4.79	24.21	h_g #7	1460	4.86	24.53	h_g #7
a_g	1510	0.04	0.23	a_g #2	1510	0.05	0.25	a_g #2	1510	0.05	0.26	a_g #2
a_g	1519	0.00	0.03	g_g #6	1519	0.00	0.01	g_g #6	1519	0.00	0.00	g_g #6
a_g	1583	2.06	12.38	h_g #8	1583	1.99	11.77	h_g #8	1584	2.11	12.55	h_g #8
a_g	1589	1.20	7.33	h_g #8	1589	1.38	8.26	h_g #8	1589	1.25	7.49	h_g #8

Table S4: Analysis of the multimode JT problem of C_{60}^- in C_{2h} conformation by the LS totally symmetric modes in the harmonic approximation. Frequencies (ν_k) of the selected normal modes are in cm^{-1} as obtained from DFT calculations. The contributions of the normal mode to the JT distortion (c_k) and the energy stabilization (E_k) are given in %. The origin of the normal mode relative to the HS normal mode is given. The origin of the LS normal mode relative to the HS normal mode is given

LS irrep	^2A_u (C_{2h})				^2B_u (C_{2h})			
	ν_k	c_k	E_k	Origin	ν_k	c_k	E_k	Origin
a_g	261	7.14	1.19	h_g #1	27	0.06	0.00	h_g #1, h_g #2
a_g	263	0.32	0.05	h_g #1	263	0.17	0.03	h_g #1
a_g	264	25.83	4.41	h_g #1	263	34.87	6.03	h_g #1
a_g	424	29.96	13.23	h_g #2	297	0.39	0.09	h_g #1, h_g #2
a_g	433	8.73	4.02	h_g #2	425	34.70	15.66	h_g #2
a_g	435	0.15	0.07	h_g #2	434	2.43	1.14	h_g #2
a_g	482	0.00	0.00	g_g #1	480	0.02	0.01	g_g #1
a_g	484	0.01	0.00	g_g #1	483	0.00	0.00	g_g #1
a_g	500	0.40	0.24	a_g #1	500	0.27	0.17	a_g #1
a_g	555	0.01	0.00	t_{2g} #1	553	0.00	0.00	g_g #2, t_{2g} #1
a_g	566	0.00	0.00	g_g #2, t_{1g} #1	556	0.01	0.01	t_{2g} #1, g_g #2
a_g	571	0.00	0.00	g_g #2, t_{1g} #1	570	0.00	0.00	t_{1g} #1
a_g	577	0.00	0.00	g_g #2, t_{1g} #1	573	0.01	0.00	h_g #3, g_g #2
a_g	707	0.66	0.81	h_g #3	573	0.00	0.00	g_g #2, h_g #3
a_g	707	3.64	4.48	h_g #3	707	0.61	0.76	h_g #3
a_g	708	7.19	8.84	h_g #3	708	10.70	13.40	h_g #3
a_g	754	0.01	0.01	t_{2g} #2	744	0.01	0.01	g_g #3
a_g	759	0.00	0.00	g_g #3	756	0.01	0.01	g_g #3
a_g	766	0.00	0.00	g_g #3, t_{2g} #3	765	0.01	0.02	h_g #4, t_{2g} #2, t_{2g} #3
a_g	787	4.79	7.28	h_g #4	766	0.00	0.00	t_{2g} #2, h_g #4, t_{2g} #3
a_g	789	0.01	0.01	h_g #4	787	4.97	7.68	h_g #4
a_g	789	0.22	0.33	h_g #4	789	0.01	0.02	h_g #4, g_g #3
a_g	801	0.00	0.00	t_{2g} #3, g_g #3	801	0.00	0.00	t_{2g} #3
a_g	831	0.00	0.00	t_{1g} #2	831	0.00	0.00	t_{1g} #2
a_g	1114	0.11	0.34	h_g #5, g_g #4	1022	0.00	0.00	g_g #4, h_g #5
a_g	1119	0.00	0.00	g_g #4, h_g #5	1115	0.18	0.56	h_g #5
a_g	1124	1.91	5.91	h_g #5, g_g #4	1117	0.02	0.06	g_g #4, h_g #5

a_g	1130	0.00	0.00	h_g #5, g_g #4	1124	1.85	5.81	h_g #5, g_g #4
a_g	1131	0.05	0.14	h_g #5, g_g #4	1130	0.01	0.02	h_g #5, g_g #4
a_g	1271	0.62	2.47	h_g #6	1201	0.01	0.04	h_g #6, h_g #5, g_g #4
a_g	1277	0.06	0.24	h_g #6	1272	0.68	2.74	h_g #6
a_g	1279	0.00	0.00	h_g #6	1279	0.02	0.07	h_g #6
a_g	1290	0.00	0.00	t_{1g} #3	1301	0.00	0.00	t_{1g} #3
a_g	1331	0.01	0.05	g_g #5	1311	0.00	0.00	h_g #6, h_g #7, t_{1g} #3
a_g	1335	0.00	0.00	g_g #5	1327	0.01	0.05	g_g #5
a_g	1357	0.00	0.00	t_{2g} #4	1334	0.00	0.01	g_g #5
a_g	1447	0.17	0.85	h_g #7	1357	0.00	0.00	t_{2g} #4
a_g	1451	0.00	0.00	h_g #7	1451	0.04	0.21	h_g #7
a_g	1461	4.75	24.84	h_g #7	1461	4.73	25.20	h_g #7
a_g	1510	0.00	0.02	a_g #2	1510	0.01	0.07	a_g #2
a_g	1519	0.00	0.00	g_g #6	1518	0.00	0.00	g_g #6
a_g	1520	0.00	0.02	g_g #6	1519	0.00	0.01	g_g #6
a_g	1583	0.02	0.11	h_g #8	1539	0.00	0.03	h_g #8, h_g #7
a_g	1583	2.05	12.60	h_g #8	1583	0.68	4.27	h_g #8
a_g	1589	1.19	7.40	h_g #8	1587	2.51	15.79	h_g #8