Supporting Information for:

Treatment of the Multimode Jahn-Teller Problem in Small Aromatic Radicals

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Supporting Information Available

Table S1: Analysis of the multimode JT problem in $C_5H_5^{\cdot}$ by the LS totally symmetric normal modes in harmonic approximation. Frequencies of normal modes are in cm^{-1} as obtained from DFT calculations; contribution of the normal mode $\vec{Q}_k$ to the $\vec{R}_{JT}$ is given by c_k in %; E_k energy contribution of $\vec{Q}_k$ to the E_{JT} in %

$\vec{Q}_k$	$\tilde{\nu}_k$ in C_{2v}	Assignement	HS-irrep	c_k	E_k
1	831	C−C−C bend	e_2'	0.2419	247.5
2	937	C−C−H bend	e_1'	0.0621	30.9
3	1040	C−C−H bend	e_2'	0.5218	247.9
4	1127	breathing	a_1'	0.0008	1.6
5	1349	C−C stretch	e_1'	0.0339	43.8
6	1482	C−C stretch	e_2'	0.1393	665.3
7	3120	C−H stretch	e_2'	0.0002	0.5
8	3140	C−H stretch	e_1'	0.0001	0.1
9	3165	C−H stretch	a_1'	0.0001	0.1

Table S2: Analysis of the multimode JT problem in $C_6H_6^{+}$ by the LS totally symmetric normal modes in harmonic approximation. Frequencies of normal modes are in cm^{-1} as obtained from DFT calculations; contribution of the normal mode $\vec{Q}_k$ to the $\vec{R}_{JT}$ is given by c_k in %; E_k energy contribution of $\vec{Q}_k$ to the E_{JT} in %

$\vec{Q}_k$	$\tilde{\nu}_k$ in D_{2h}	Assignment	HS-irrep	c_k	E_k
1	591	C−C−C bend	e_{2g}	51.99	34.32
2	976	breathing	a_{1g}	0.95	1.62
3	1166	C−C−H bend	e_{2g}	34.63	16.99
4	1556	C−C stretch	e_{2g}	12.40	46.99
5	3109	C−H stretch	e_{2g}	0.01	0.06
6	3127	C−H stretch	a_{1g}	0.00	0.00

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Table S3: Analysis of the multimode JT problem in $C_7H_7^{\cdot}$ by the LS totally symmetric normal modes in harmonic approximation. Frequencies of normal modes are in cm^{-1} as obtained from DFT calculations; contribution of the normal mode $\vec{Q}_\mathrm{k}$ to the $\vec{R}_\mathrm{JT}$ is given by c_k in %; E_k energy contribution of $\vec{Q}_\mathrm{k}$ to the E_JT in %

$\vec{Q}_\mathrm{k}$	$\tilde{\nu}_\mathrm{k}$ in C_{2v}	Assignment	HS-irrep	c_k	E_k
1	434	C−C−C bend	e_2'	0.00	0.00
2	852	breathing	a_1'	0.76	0.28
3	894	C−C−C bend	e_3'	5.31	1.87
4	957	C−C−H bend	e_1'	2.90	0.48
5	1161	C−C−H bend	e_2'	0.22	0.03
6	1234	C−C−H bend	e_3'	30.53	3.92
7	1421	C−C−H bend	e_1'	10.49	2.71
8	1516	C−C stretch	e_2'	4.47	2.66
9	1611	C−C stretch	e_3'	44.07	87.55
10	3050	C−H stretch	e_3'	0.09	0.07
11	3055	C−H stretch	e_2'	0.15	0.12
12	3086	C−H stretch	e_1'	0.29	0.24
13	3099	C−H stretch	a_1'	0.07	0.06

Table S4: Analysis of the multimode JT problem in $C_6H_6^-$, $D_{6h} \longrightarrow D_{2h}$ distortion, by the LS totally symmetric normal modes in harmonic approximation. Frequencies of normal modes are in cm^{-1} as obtained from DFT calculations; contribution of the normal mode $\vec{Q}_\mathrm{k}$ to the $\vec{R}_\mathrm{JT}$ is given by c_k in %; E_k energy contribution of $\vec{Q}_\mathrm{k}$ to the E_JT in %

$\vec{Q}_\mathrm{k}$	$\tilde{\nu}_\mathrm{k}$ in D_{2h}	Assignment	HS-irrep	c_k	E_k
1	604	C−C−C bend	e_{2g}	9.58	5.21
2	959	breathing	a_{1g}	2.20	2.84
3	1093	C−C−H bend	e_{2g}	64.69	22.21
4	1498	C−C stretch	e_{2g}	23.27	69.16
5	2995	C−H stretch	e_{2g}	0.22	0.53
6	3076	C−H stretch	a_{1g}	0.01	0.02

Table S5: Analysis of the multimode JT problem in $C_6H_6^-$, $D_{6h} \longrightarrow C_{2v}$ distortion, by the LS totally symmetric normal modes in harmonic approximation. Frequencies of normal modes are in cm^{-1} as obtained from DFT calculations; contribution of the normal mode $\vec{Q}_\mathrm{k}$ to the $\vec{R}_\mathrm{JT}$ is given by c_k in %; E_k energy contribution of $\vec{Q}_\mathrm{k}$ to the E_JT in %

$\vec{Q}_\mathrm{k}$	$\tilde{\nu}_\mathrm{k}$ in D_{2h}	Assignment	HS-irrep	c_k	E_k
1	320	out-of plane	e_{2u}	90.87	51.19
2	529	C−H wagging	b_{2u}	2.38	1.47
3	578	C−C−C bend	e_{2g}	1.27	3.48
4	718	C−H wagging	b_{2u}	0.08	0.11
5	878	breathing	a_{1g}	0.22	1.87
6	1112	C−C−H bend	e_{2g}	3.88	10.42
7	1531	C−C stretch	e_{2g}	0.97	25.86
8	2947	C−H stretch	e_{2g}	0.26	4.77
9	3015	C−H stretch	a_{1g}	0.04	0.78