Supporting information for Rationalization of photo-detachment spectra of indenyl anion ($C_9H_7^-$) from the perception of vibronic coupling theory

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TABLE S1. Harmonic frequencies [in cm^{-1} (eV)] of the vibrational modes of ground state equilibrium structures of indenyl anion and indenyl radical calculated at MP2 level of theory using cc-pvtz basis set are given in this table.

Vibrational Mode(symmetry)	Anion Frequency(ω_i)	Neutral Frequency(ω_i)
$\nu_1(a_1)$	545 (0.0676)	541.90
$\nu_2(a_1)$	744 (0.0923)	752.78
$\nu_3(a_1)$	859 (0.1065)	888.08
$\nu_4(a_1)$	1017 (0.1261)	1035.16
$\nu_5(a_1)$	1053 (0.1305)	1119.42
$\nu_6(a_1)$	1146 (0.1421)	1173.27
$\nu_7(a_1)$	1287 (0.1596)	1277.01
$\nu_8(a_1)$	1374 (0.1703)	1464.00
$\nu_9(a_1)$	1448 (0.1795)	1512.84
$\nu_{10}(a_1)$	1559 (0.1932)	1572.97
$\nu_{11}(a_1)$	1594 (0.1976)	1635.07
$\nu_{12}(a_1)$	3143 (0.3897)	3209.68
$\nu_{13}(a_1)$	3175 (0.3937)	3233.74
$\nu_{14}(a_1)$	3187 (0.3951)	3256.70
$\nu_{15}(a_1)$	3219 (0.3991)	3285.35
$\nu_{16}(b_2)$	382 (0.0474)	381.43
$\nu_{17}(b_2)$	588 (0.0728)	632.30
$\nu_{18}(b_2)$	881 (0.1092)	894.77
$\nu_{19}(b_2)$	1042 (0.1292)	1062.20
$\nu_{20}(b_2)$	1115 (0.1383)	1153.63
$\nu_{21}(b_2)$	1194 (0.1481)	1207.54
$\nu_{22}(b_2)$	1238 (0.1535)	1267.15
$\nu_{23}(b_2)$	1359 (0.1684)	1387.12
$\nu_{24}(b_2)$	1462 (0.1813)	1427.56
$\nu_{25}(b_2)$	1504 (0.1865)	1521.23
$\nu_{26}(b_2)$	1643 (0.2037)	3087.16
$\nu_{27}(b_2)$	3138 (0.3891)	3207.36
$\nu_{28}(b_2)$	3166 (0.3926)	3222.32
$\nu_{29}(b_2)$	3209 (0.3979)	3279.79
$\nu_{30}(b_1)$	210 (0.0260)	196.02
$\nu_{31}(b_1)$	405 (0.0502)	408.86
$\nu_{32}(b_1)$	572 (0.0709)	555.88
$\nu_{33}(b_1)$	661 (0.0819)	752.79
$\nu_{34}(b_1)$	704 (0.0872)	784.11
$\nu_{35}(b_1)$	773 (0.0958)	888.09
$\nu_{36}(b_1)$	836 (0.1036)	894..78
$\nu_{37}(a_2)$	229 (0.02839)	242.87
$\nu_{38}(a_2)$	248 (0.03074)	552.67
$\nu_{39}(a_2)$	602 (0.07463)	711.03
$\nu_{40}(a_2)$	655 (0.08120)	744.47
$\nu_{41}(a_2)$	773 (0.0958)	883.45
$\nu_{42}(a_2)$	867 (0.1074)	949.69

TABLE S2. Higher-order Hamiltonian parameters of totally symmetric vibrational modes.

Mode	C	D	C	D
	X^2A_2		A^2B_1	
ν_2	-0.0002	0.0000	0.0000	0.0000
ν_8	0.0011	0.0000	0.0036	0.0000
ν_{10}	-0.0007	0.0000	-0.0009	0.0000
ν_{11}	-0.0207	0.0000	0.0137	0.0000
	B^2A_2		C^2B_1	
ν_5	-0.0026	0.0000	-0.0003	0.00000
ν_6	-0.0004	0.0000	0.0041	0.00000
ν_8	-0.0017	0.0000	0.0001	0.00000
ν_{12}	0.0000	0.0000	-0.0005	0.00000

TABLE S3. Normal modes combination , size of primitive and single partition function(SPF)for coupled two and four states nuclear dynamics (time-dependent) of indenyl using MCTDH approach [1]

Normal modes combination	Primitive basis	SPF basis	Figure
(ν_1)	(18)	[9,9]	
(ν_{11}, ν_{24})	(14, 15)	[8,8]	
(ν_3, ν_{17})	(11, 11)	[6,6]	Fig. 8
(ν_{10}, ν_{16}, ν_{19}, ν_{20}, ν_{25})	(10, 9, 9, 10, 10)	[5,5]	
(ν_5, ν_6, ν_7, ν_{26})	(7, 7, 7, 7)	[3,3]	
(ν_1, ν_{11}, ν_{24})	(14, 14, 14)	[8, 8, 8, 8]	
(ν_{17}, ν_{25}, ν_{26})	(11,11,11)	[6, 6, 6, 6]	
(ν_5, ν_{10}, ν_{16}, ν_{19}, ν_{20})	(10, 10, 10, 10, 10)	[5, 5, 5, 5]	Fig.9
(ν_3, ν_4)	(10, 10)	[5, 5, 5, 5]	
(ν_6, ν_7, ν_8)	(8, 8, 8)	[3, 3, 3, 3]	
(ν_9, ν_{21})	(6, 6)	[2, 2, 2, 2]	

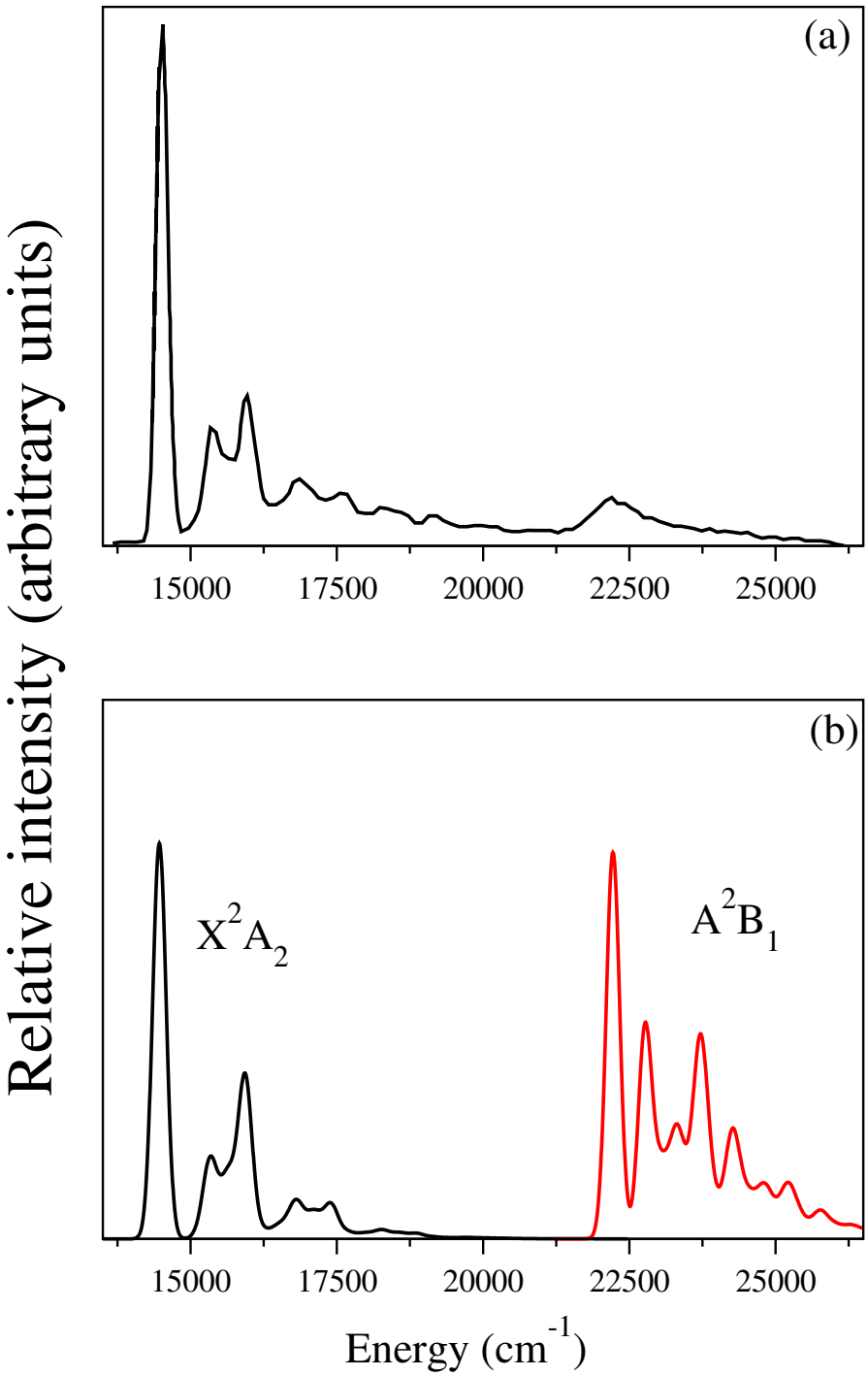

FIG. S1. Comparison of spectrum obtained from Franck-Condon simulation (panel b) with experimental observation of overview of SEVI spectra of the $\tilde{X}^2A_2$ and $\tilde{A}^2B_1$ state of indenyl (panel a). Franck-Condon simulations are performed on the basis of ground state energy minimum structure of indenyl anion and ground and first excited state energy minimum structures of indenyl radical. The calculations of these electronic structures are performed employing density functional theory.

BIBLIOGRAPHY

[1] G.A. Worth, M.H. Beck, A. Jäckle, H.-D. Meyer, *The mctdh package, Version 8.4, (2007), University of Heidelberg, Heidelberg, Germany. See:http://mctdh.uni-hd.de*