SUPPLEMENTARY INFORMATION

Interaction Of Slow Electrons With Thermally Evaporated Manganese (II) Acetylacetonate Complexes

Janina Kopyra[1], Franck Rabilloud[2], Hassan Abdoul-Carime[3*]

[1] *Siedlce University of Natural Sciences and Humanities, Faculty of Exact and Natural Sciences, 3 Maja 54, 08-110 Siedlce, Poland*

[2] *Univ Lyon, Univ Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, F-69622, Villeurbanne, France*

[3] *Université de Lyon, F-69003, Lyon, France; Université Lyon 1, Villeurbanne; CNRS/IN2P3, UMR5822, Institut de Physique des 2 Infinis*

S1. Molecular Constants

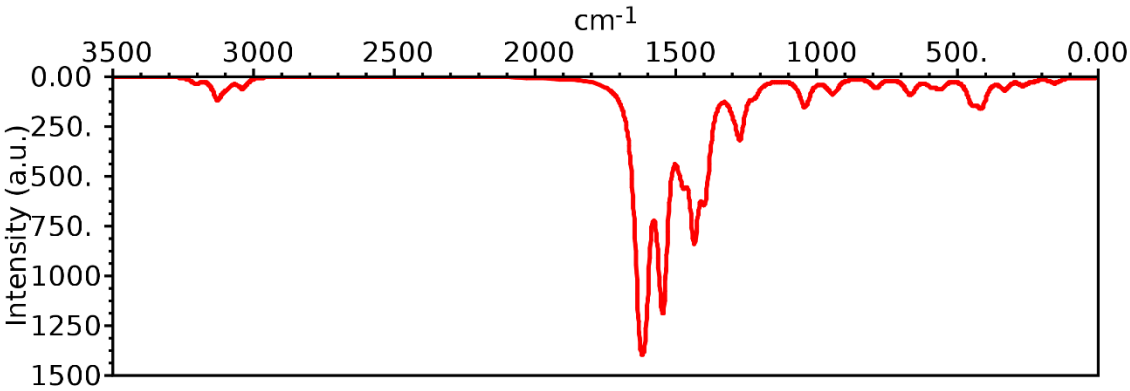
The dipole moment (D), quadrupole moment (Q_{xx},Q_{yy},Q_{zz}, and Q_{xy},Q_{xz},Q_{yz} in D.Å), polarizability (α_{xx}, α_{yy}, α_{zz} in Bohr^3), and rotational constants B_x, B_y, B_z (GHz). The magnitude of the polarizability and quadrupole moment can be estimated via $< A > \sqrt{(A_{xx}^2 + A_{yy}^2 + A_{zz}^2)}$. Note that for the $Mn(acac)_3$, we first diagonalize the Q matrix prior to averaging the trace.

		$Mn(acac)_2$ (D_{2d})	$Mn(acac)_3$ (C_1)
Dipole moment (D)		0.0	1.0446
Quadrupole Moment (D.Å)	Q_{xx}	-89.4789	-126.464
	Q_{yy}	-88.2445	-120.0745
	Q_{zz}	-96.6031	-135.7288
	Q_{xy}	8.3525	0.8306
	Q_{xz}	0.0	2.6533
	Q_{yz}	0.0	-0.2809
Polarizability (Bohr^3)		190.539	254.679
		150.416	258.453
		150.247	234.677
Rotational constants (GHz)		0.82516	0.26449477
		0.26875	0.25776180
		0.26860	0.19126338

S2. Vibrational Levels of the neutral D_{2d}-symmetry Mn(II)(acac)$_2$

Harmonic frequencies (in cm^{-1}) calculated at B3LYP/Def2-TZVP level and the option "UltraFineGrid" for numerical integrations. The infrared spectrum is also showed.

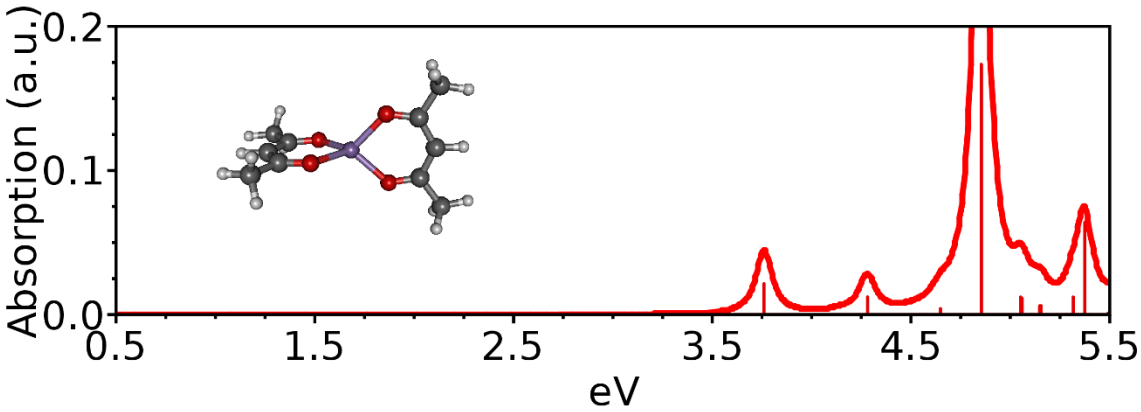
Frequencies --	27.0975	27.1126	29.3103
Frequencies --	86.9526	86.9862	97.7703
Frequencies --	98.2685	122.1054	122.1558
Frequencies --	123.1705	138.8497	151.2601
Frequencies --	163.2533	163.2615	232.9313
Frequencies --	246.0308	253.0885	253.2902
Frequencies --	294.6363	409.3413	409.3533
Frequencies --	428.5442	450.6556	554.1099
Frequencies --	554.1430	576.5221	576.6076
Frequencies --	664.0187	665.5975	678.7484
Frequencies --	678.7493	801.5792	801.6014
Frequencies --	941.6769	941.6860	953.4375
Frequencies --	953.5001	1038.0717	1038.0743
Frequencies --	1041.7317	1042.5872	1047.7033
Frequencies --	1047.7043	1060.1762	1060.2216
Frequencies --	1227.1782	1227.1883	1281.2653
Frequencies --	1284.4874	1395.9606	1395.9615
Frequencies --	1397.1372	1397.2073	1431.4819
Frequencies --	1431.5312	1473.3570	1473.4424
Frequencies --	1474.0501	1474.0533	1477.8491
Frequencies --	1478.4339	1493.8634	1493.8798
Frequencies --	1552.3208	1552.3299	1606.3579
Frequencies --	1627.0600	3040.6361	3040.6545
Frequencies --	3040.7554	3040.7769	3095.3121
Frequencies --	3095.3221	3095.4748	3095.4757
Frequencies --	3131.3306	3131.4372	3131.6813
Frequencies --	3131.7001	3204.4289	3204.5140



S3. Excited states of the neutral D_{2d}-symmetry Mn(II)(acac)$_2$

Calculations at TDDFT/B3LYP/aug-cc-pvtz level.

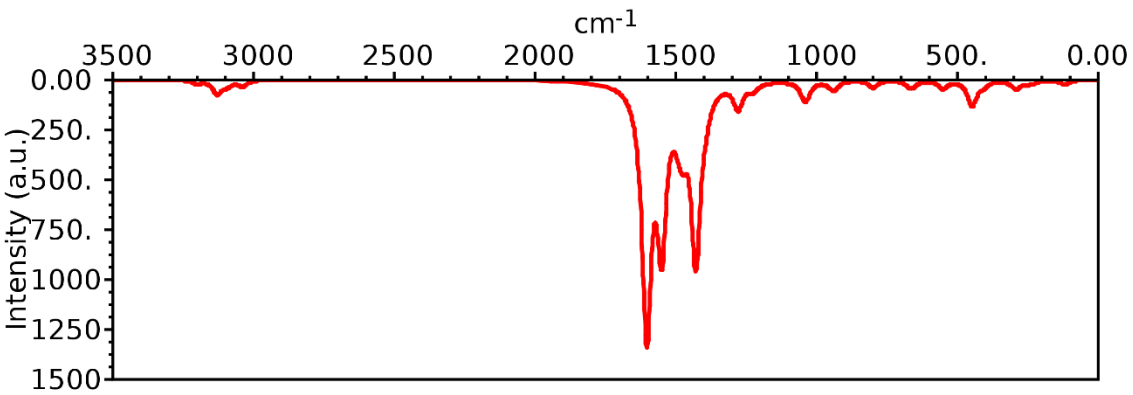
		(eV)	(nm)	oscillator strength (a.u.)
Excited State	1:	2.9687 eV	417.64 nm	f=0.0000
Excited State	2:	2.9687 eV	417.63 nm	f=0.0000
Excited State	3:	3.2214 eV	384.88 nm	f=0.0001
Excited State	4:	3.2216 eV	384.86 nm	f=0.0001
Excited State	5:	3.7642 eV	329.38 nm	f=0.0221
Excited State	6:	3.7644 eV	329.36 nm	f=0.0220
Excited State	7:	4.1434 eV	299.24 nm	f=0.0007
Excited State	8:	4.1434 eV	299.23 nm	f=0.0007
Excited State	9:	4.2831 eV	289.47 nm	f=0.0128
Excited State	10:	4.2834 eV	289.46 nm	f=0.0127
Excited State	11:	4.5510 eV	272.43 nm	f=0.0000
Excited State	12:	4.5629 eV	271.72 nm	f=0.0002
Excited State	13:	4.5630 eV	271.72 nm	f=0.0002
Excited State	14:	4.5779 eV	270.83 nm	f=0.0000
Excited State	15:	4.6515 eV	266.55 nm	f=0.0043
Excited State	16:	4.6540 eV	266.40 nm	f=0.0045
Excited State	17:	4.8548 eV	255.38 nm	f=0.1739
Excited State	18:	4.8552 eV	255.37 nm	f=0.1742
Excited State	19:	4.9691 eV	249.51 nm	f=0.0000
Excited State	20:	5.0582 eV	245.12 nm	f=0.0122
Excited State	21:	5.0603 eV	245.01 nm	f=0.0121
Excited State	22:	5.1107 eV	242.60 nm	f=0.0000
Excited State	23:	5.1141 eV	242.43 nm	f=0.0004
Excited State	24:	5.1143 eV	242.43 nm	f=0.0005
Excited State	25:	5.1548 eV	240.52 nm	f=0.0067
Excited State	26:	5.1551 eV	240.51 nm	f=0.0067
Excited State	27:	5.2417 eV	236.53 nm	f=0.0000
Excited State	28:	5.2804 eV	234.80 nm	f=0.0000
Excited State	29:	5.2805 eV	234.79 nm	f=0.0000
Excited State	30:	5.3037 eV	233.77 nm	f=0.0000



S4. Vibrational Levels of the neutral C_1-symmetry Mn(III)(acac)$_3$

Harmonic frequencies (in cm^{-1}) calculated at B3LYP/Def2-TZVP level and the option "UltraFineGrid" for numerical integrations. The infrared spectrum is also showed.

Frequencies --	21.2025	23.3277	30.4756
Frequencies --	41.2737	44.2339	45.5385
Frequencies --	60.8599	61.7540	84.3338
Frequencies --	95.1311	107.1536	107.4718
Frequencies --	135.5563	140.4658	157.2103
Frequencies --	159.3928	160.8868	164.4892
Frequencies --	164.9301	171.1888	183.8328
Frequencies --	190.1394	198.9359	233.8508
Frequencies --	234.4916	248.0338	260.0153
Frequencies --	270.5295	333.1120	334.8741
Frequencies --	408.7235	410.5165	414.9672
Frequencies --	427.4002	438.8802	453.2361
Frequencies --	555.0035	563.4780	571.8199
Frequencies --	573.4587	575.2375	594.5469
Frequencies --	663.9877	668.4834	676.7616
Frequencies --	677.6796	678.3145	684.8158
Frequencies --	790.8960	790.9585	794.1026
Frequencies --	939.0203	940.2987	947.2801
Frequencies --	954.4365	955.7325	969.0266
Frequencies --	1035.9756	1036.5811	1039.7340
Frequencies --	1042.7493	1044.6249	1045.1177
Frequencies --	1045.3431	1048.1646	1051.7680
Frequencies --	1059.2396	1059.6071	1060.6122
Frequencies --	1218.1602	1222.6802	1223.0064
Frequencies --	1275.0982	1280.1206	1301.8591
Frequencies --	1391.5875	1391.6642	1395.3085
Frequencies --	1397.3960	1398.1375	1398.2509
Frequencies --	1401.7762	1433.7730	1437.3825
Frequencies --	1472.4450	1472.5021	1472.6648
Frequencies --	1473.0917	1474.4934	1474.6170
Frequencies --	1476.8269	1477.4587	1478.2981
Frequencies --	1486.9176	1494.8627	1497.0507
Frequencies --	1545.0633	1546.0430	1557.7811
Frequencies --	1610.7326	1631.6410	1650.6313
Frequencies --	3041.0041	3041.0162	3041.0747
Frequencies --	3041.1420	3044.3520	3044.3949
Frequencies --	3095.8492	3095.9207	3098.2627
Frequencies --	3098.2772	3100.7133	3100.8184
Frequencies --	3127.2069	3127.2571	3131.4770
Frequencies --	3131.5184	3135.7265	3135.8293
Frequencies --	3205.7776	3205.8786	3217.0972



S5. Excited states of the neutral D_3-symmetry Mn(III)(acac)$_3$

Calculations at TDDFT/B3LYP/aug-cc-pvtz level

		(eV)		(nm)		oscillator strength (a.u.)
Excited State	1:	0.9532	ev	1300.77	nm	f=0.0021
Excited State	2:	2.1702	ev	571.30	nm	f=0.0009
Excited State	3:	2.3418	ev	529.43	nm	f=0.0018
Excited State	4:	2.6511	ev	467.67	nm	f=0.0004
Excited State	5:	2.8258	ev	438.76	nm	f=0.0028
Excited State	6:	2.9178	ev	424.93	nm	f=0.0041
Excited State	7:	2.9770	ev	416.48	nm	f=0.0000
Excited State	8:	3.0166	ev	411.01	nm	f=0.0006
Excited State	9:	3.2556	ev	380.83	nm	f=0.0001
Excited State	10:	3.2845	ev	377.48	nm	f=0.0016
Excited State	11:	3.3266	ev	372.71	nm	f=0.0293
Excited State	12:	3.3365	ev	371.60	nm	f=0.0042
Excited State	13:	3.4086	ev	363.74	nm	f=0.0006
Excited State	14:	3.4388	ev	360.54	nm	f=0.0001
Excited State	15:	3.4417	ev	360.24	nm	f=0.0034
Excited State	16:	3.5068	ev	353.55	nm	f=0.0000
Excited State	17:	3.5842	ev	345.92	nm	f=0.0352
Excited State	18:	3.6628	ev	338.50	nm	f=0.0061
Excited State	19:	3.6684	ev	337.97	nm	f=0.0172
Excited State	20:	3.8577	ev	321.39	nm	f=0.0023
Excited State	21:	3.8682	ev	320.53	nm	f=0.0009
Excited State	22:	3.9118	ev	316.95	nm	f=0.0003
Excited State	23:	3.9411	ev	314.59	nm	f=0.0109
Excited State	24:	3.9565	ev	313.37	nm	f=0.0001
Excited State	25:	3.9701	ev	312.29	nm	f=0.0064
Excited State	26:	4.0056	ev	309.53	nm	f=0.0056
Excited State	27:	4.0260	ev	307.96	nm	f=0.0055
Excited State	28:	4.0462	ev	306.42	nm	f=0.0209
Excited State	29:	4.1805	ev	296.58	nm	f=0.0013
Excited State	30:	4.1965	ev	295.45	nm	f=0.0554
Excited State	31:	4.2475	ev	291.90	nm	f=0.0005
Excited State	32:	4.2931	ev	288.80	nm	f=0.0126
Excited State	33:	4.4002	ev	281.77	nm	f=0.0263
Excited State	34:	4.4317	ev	279.77	nm	f=0.0014
Excited State	35:	4.4340	ev	279.62	nm	f=0.0005
Excited State	36:	4.4472	ev	278.79	nm	f=0.0026
Excited State	37:	4.5129	ev	274.73	nm	f=0.0067
Excited State	38:	4.5206	ev	274.27	nm	f=0.0030
Excited State	39:	4.5782	ev	270.81	nm	f=0.0125
Excited State	40:	4.6000	ev	269.53	nm	f=0.0125
Excited State	41:	4.6754	ev	265.18	nm	f=0.0078
Excited State	42:	4.6830	ev	264.75	nm	f=0.0009
Excited State	43:	4.7085	ev	263.32	nm	f=0.0009
Excited State	44:	4.7163	ev	262.89	nm	f=0.0016
Excited State	45:	4.7711	ev	259.87	nm	f=0.0024
Excited State	46:	4.7827	ev	259.24	nm	f=0.0038
Excited State	47:	4.7957	ev	258.53	nm	f=0.0087
Excited State	48:	4.7964	ev	258.49	nm	f=0.0006
Excited State	49:	4.8126	ev	257.62	nm	f=0.0002
Excited State	50:	4.8530	ev	255.48	nm	f=0.0005
Excited State	51:	4.8788	ev	254.13	nm	f=0.0071
Excited State	52:	4.9044	ev	252.80	nm	f=0.0009
Excited State	53:	4.9178	ev	252.11	nm	f=0.0230
Excited State	54:	4.9541	ev	250.27	nm	f=0.0345
Excited State	55:	4.9729	ev	249.32	nm	f=0.0001
Excited State	56:	5.0118	ev	247.39	nm	f=0.0091
Excited State	57:	5.0217	ev	246.90	nm	f=0.0083
Excited State	58:	5.0333	ev	246.33	nm	f=0.0080
Excited State	59:	5.0465	ev	245.68	nm	f=0.0132
Excited State	60:	5.0497	ev	245.53	nm	f=0.0147
Excited State	61:	5.0692	ev	244.58	nm	f=0.1289
Excited State	62:	5.0752	ev	244.29	nm	f=0.0042
Excited State	63:	5.1046	ev	242.89	nm	f=0.0073

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Excited State  64:      5.1412 eV  241.16 nm  f=0.0005
Excited State  65:      5.1602 eV  240.27 nm  f=0.0006
Excited State  66:      5.1759 eV  239.54 nm  f=0.0091
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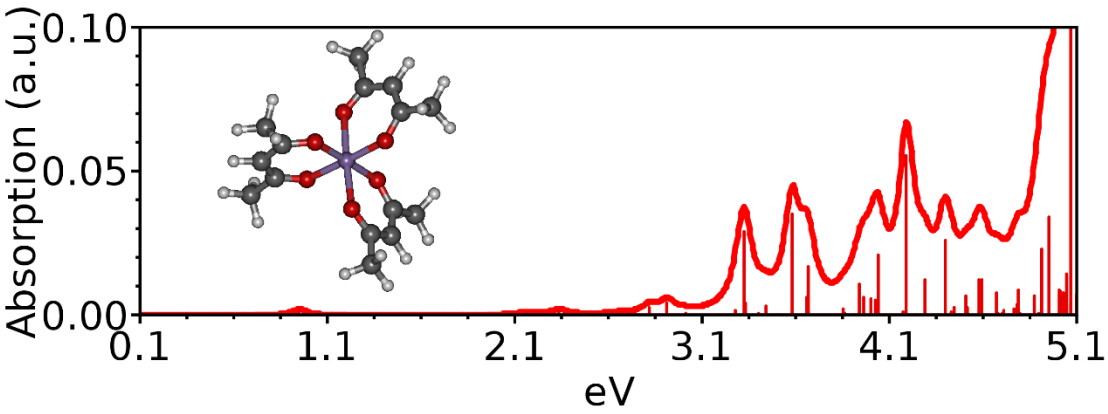
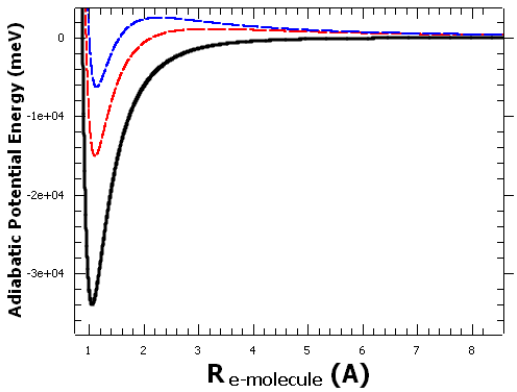
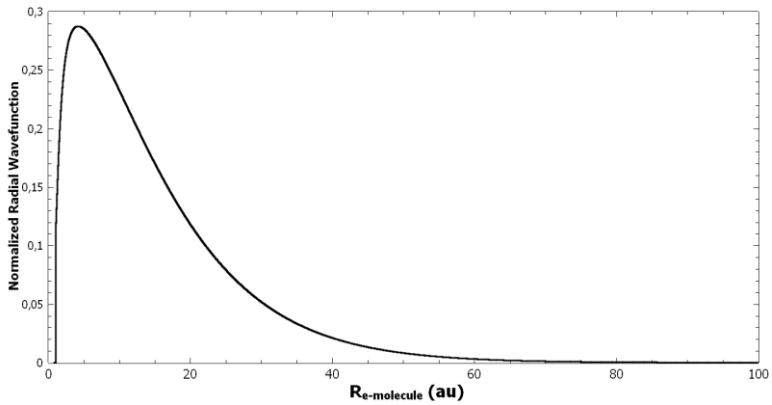


S6. Adiabatic Potential Curve, Normalized Radial wave function, l dependency of the binding energy

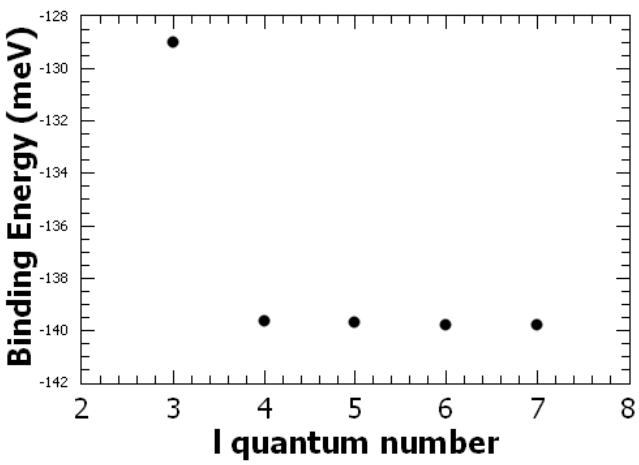
Adiabatic Potential Curve (black is the lowest, followed by red and blue). $R_{e\text{-molecule}}$ is expressed in Angströem.



Normalized Radial Wave Function. The distance $R_{e\text{-molecule}}$ is expressed in atomic unit (au)

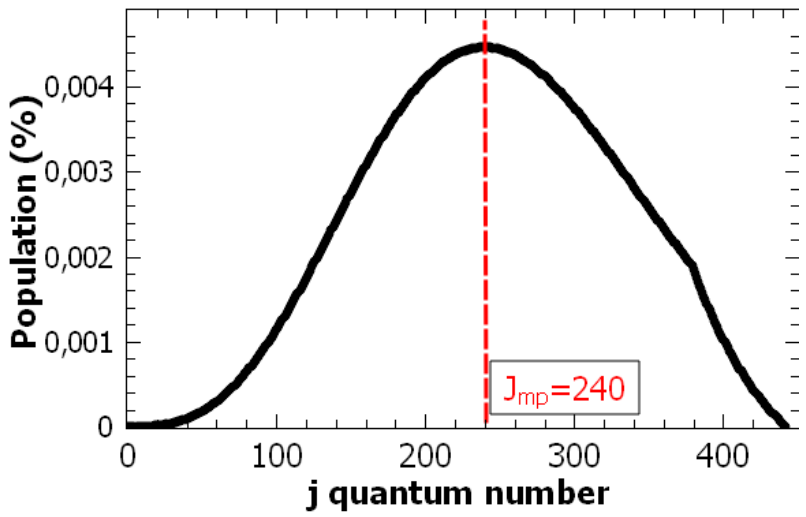
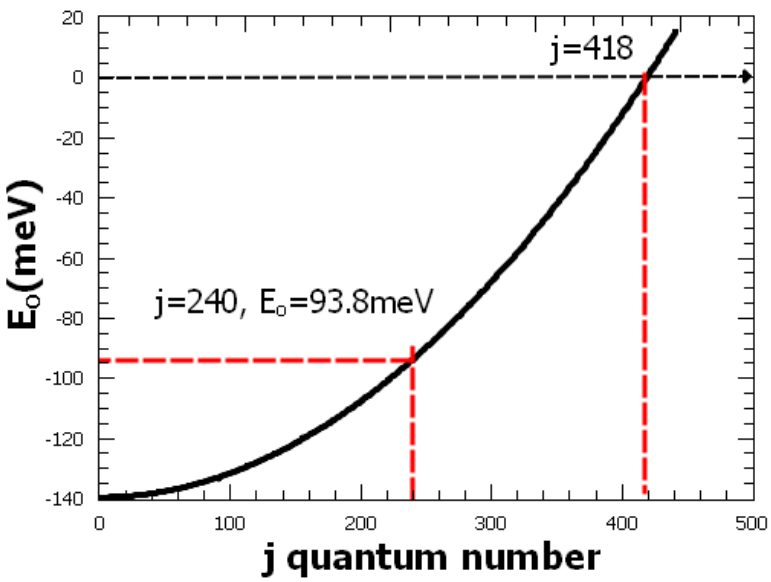


"l" dependency of the Binding Energy from the semi-empirical model



S7 : (a) multipole bound (J, k=0) states and (b) Population of accessible bound « j » states following the Boltzmann distribution.

(a) Population of accessible bound « j » states. For each « j » state, the population of accessible states is integrated over all possible « k » states, i.e., for which the electron is still bound to the molecule.. The most probable rotational state is J_{mp}=240.



(b) . **Multipole bound (J, k=0) states.** The last bound « J » state (i.e. E<0) is obtained for J=418.