

## Electronic Supplementary Information (ESI) for: A Molecular Quantum Switch Based on Tunneling in Meta-D-phenol C<sub>6</sub>H<sub>4</sub>DOH

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Table A1: Lowest ab initio (ai) and adjusted (adj) adiabatic channel potentials ( $E/(hc \text{ cm}^{-1})$ ) as a function of the torsional coordinate ( $\varphi/^\circ$ ) for meta-D-phenol

$\varphi$	$E_{\text{ai}}/(hc)$	$E_{\text{adj}}/(hc)$	$\varphi$	$E_{\text{ai}}/(hc)$	$E_{\text{adj}}/(hc)$	$\varphi$	$E_{\text{ai}}/(hc)$	$E_{\text{adj}}/(hc)$
-90.0	1199.65	1199.99	35.0	412.18	412.52	160.0	166.13	165.79
-85.0	1192.60	1192.94	40.0	513.49	513.83	165.0	99.71	99.37
-80.0	1170.22	1170.56	45.0	616.91	617.25	170.0	48.44	48.10
-75.0	1131.46	1131.80	50.0	719.58	719.92	175.0	14.82	14.48
-70.0	1076.64	1076.98	55.0	818.35	818.69	180.0	1.66	1.32
-65.0	1007.84	1008.18	60.0	910.15	910.49	185.0	10.48	10.14
-60.0	927.41	927.75	65.0	992.66	993.00	190.0	40.23	39.89
-55.0	837.30	837.64	70.0	1063.95	1064.29	195.0	88.21	87.87
-50.0	739.69	740.03	75.0	1121.76	1122.10	200.0	151.77	151.43
-45.0	637.54	637.88	80.0	1163.82	1164.16	205.0	228.80	228.46
-40.0	534.04	534.38	85.0	1189.39	1189.73	210.0	316.92	316.58
-35.0	432.08	432.42	90.0	1199.66	1199.32	215.0	413.17	412.83
-30.0	334.49	334.83	95.0	1192.72	1192.38	220.0	514.40	514.06
-25.0	244.39	244.73	100.0	1170.44	1170.10	225.0	617.73	617.39
-20.0	164.86	165.20	105.0	1131.78	1131.44	230.0	720.31	719.97
-15.0	98.34	98.68	110.0	1077.04	1076.70	235.0	819.00	818.66
-10.0	46.95	47.29	115.0	1008.32	1007.98	240.0	910.73	910.39
-5.0	13.26	13.60	120.0	927.97	927.63	245.0	993.15	992.81
0.0	0.08	0.42	125.0	837.94	837.60	250.0	1064.37	1064.03
5.0	8.91	9.25	130.0	740.41	740.07	255.0	1122.10	1121.76
10.0	38.72	39.06	135.0	638.35	638.01	260.0	1164.06	1163.72
15.0	86.81	87.15	140.0	534.94	534.60	265.0	1189.53	1189.19
20.0	150.48	150.82	145.0	433.06	432.72	270.0	1199.65	1199.31
25.0	227.60	227.94	150.0	335.57	335.23			
30.0	315.82	316.16	155.0	245.57	245.23			