Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

On the Nonadiabatic Collisional Quenching of OH(A) by H_2: A Four Coupled Quasi-Diabatic State Description

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S1. The Basis Monomials

Table SI1 contains the definitions of the elementary functions comprising the basis monomials, $g^{(l)}$. Table SI2 contains the monomials, $g^{(l)}$, used in this work. Columns 2 and 3 report the type of coordinate and the R^{ij} scaling used, respectively. Column 4 reports the atoms defining the coordinate. And column 5 is the values of the parameters C_1 and C_2. Column 6 is the maximum order of the coordinate basis function.

Table SI1. Definitions of elementary functions comprising $\boldsymbol{g}^{(l)}$

Scaling Type #	Form	Description
(a) Atom-atom distance (denoted Stretch) coordinates ($r_{AB} = \|R_A - R_B\|$)		
1	$exp\left[-C_1(r_{AB} - C_2)\right]$	Morse Function
2	$exp\left[-C_1(r_{AB} - C_2)^2\right]$	Gaussian Function
3	$exp\left[-C_1(r_{AB} - C_2)\right]/r_{AB}$	Yukawa Function
4	$\tanh\left[(r_{AB} - C_2)/C_1\right]$	Hyperbolic Tangent Function
(b) Angle bend (denoted Angle) coordinates (θ_{ABC} is the ABC angle with atom B on the vertex)		
1	$\dfrac{\cos\theta_{ABC}}{1 + exp\left[C_1\left(r_{AB}^2 + r_{BC}^2 + C_2^2\right)\right]}$	Distance-scaled Cosine
(c) Out-of-plane (denoted OOP) coordinates, where triple product $\phi_{ABCD} = (R_B - R_A) \times (R_C - R_A) \cdot (R_D - R_A)$		
1	$\dfrac{C_2\,\phi_{ABCD}}{\left(r_{AB}r_{AC}r_{AD}r_{BC}r_{BD}r_{CD}\right)^{C_1}}$	Symmetric with respect to all atoms
2	$\dfrac{\phi_{ABCD}}{r_{AB}r_{AC}r_{AD}}\left\{\sum_{X=B,C,D} exp\left[-C_1(r_{AB} - C_2)^2\right]\right\}^{-1}$	Symmetric with respect to B, C, and D
(d) Dot products (denoted DP) where $\phi_{ABCD} = \dfrac{R_B - R_A}{r_{AB}} \cdot \dfrac{R_D - R_C}{r_{CD}}$		
1	$\dfrac{\phi_{ABCD}}{\sum_{X=A,B}\sum_{Y=C,D} exp\left[-C_1(r_{XY} - C_2)^2\right]}$	

Table SI2. Elementary functions of $\boldsymbol{g}^{(i)}$. Max Order indicates the maximum of function per monomial $\boldsymbol{g}^{(i)}$. Additionally, the sum of the orders of functions 1-10 and 17-18 must not exceed 2 in any monomial $\boldsymbol{g}^{(i)}$. O = 1, H^a = 2, H^b = 3, and H^c = 4.

Index	Type	Scaling	Atoms	Parameters	Max Order
1	Stretch	1	1 2	1.2 2.0	2
2	Stretch	1	1 4	1.2 2.0	2
3	Stretch	1	2 4	1.0 2.0	2
4	Stretch	1	2 3	1.0 2.0	2
5	Stretch	3	1 2	1.0 2.0	1
6	Stretch	3	1 4	1.0 2.0	1
7	Stretch	3	2 4	1.0 2.0	1
8	Stretch	3	2 3	1.0 2.0	1
9	Angle	1	2 1 3	0.2 3.0	
10	Angle	1	2 1 4	0.2 3.0	
11	OOP	2	1 2 3 4	0.2 2.5	
12	DP	1	1 2 3 4	0.2 3.0	
13	DP	1	1 4 3 2	0.2 3.0	
14	OOP	1	1 2 3 4	0.1 3.0	
15	OOP	2	4 2 3 1	0.1 3.0	
16	OOP	2	2 3 4 1	0.1 3.0	
17	Angle	1	2 4 3	0.1 3.0	
18	Angle	1	2 3 4	0.1 3.0	
19	Stretch	4	1 4	0.4 2.3	2
20	Stretch	4	1 2	0.4 2.3	2
21	Stretch	4	2 4	0.2 3.2	2
22	Stretch	4	2 3	0.2 3.2	2
23	Stretch	4	1 4	0.2 5.7	2
24	Stretch	4	1 2	0.2 5.7	2
25	Stretch	4	2 3	1.7 4.8	2
26	Stretch	4	2 4	1.7 4.8	2
27	Stretch	2	1 3	0.8 4.1	1
28	Stretch	2	1 4	0.8 4.1	1

Table SI3. Entrance channel critical point structures. First line for each species is the *ab initio* results. Distances are in Å. Angles are in degrees.

	$R(OH^a)$	$R(OH^b)$	$R(OH^c)$	$R(H^aH^b)$	$R(H^aH^c)$	$R(H^bH^c)$	$H^aOH^bH^c$	$R(OH\text{-}H_2)$
$Q_{OH+H_2}^{min}(1^2A)$			0.966	0.743				
H[d] (1)			0.966	0.744				
H[d] (2)			0.967	0.743				
H[d] (3)			0.967	0.743				
Ref. 1			0.970	0.741				
$Q_{OH+H_2}^{min}(3^2A)$			1.006	0.743				
H[d] (1)			1.006	0.742				
H[d] (2)			1.006	0.743				
H[d] (3)			1.006	0.743				
Ref. 2			1.009	0.743				
$Q_{OH-H_2}^{min}(1^2A)$	3.300	3.300	0.966	0.744	2.342	2.342	0.01	3.279
H[d] (1)	3.313	3.313	0.967	0.744	2.355	2.355	0.00	3.292
H[d] (2)	3.318	3.330	0.967	0.744	2.367	2.366	0.00	3.303
H[d] (3)	3.318	3.330	0.967	0.744	2.366	2.367	0.00	3.303
Ref. 3	3.330	3.330	0.977	0.744			0.00	3.309
$Q_{OH-H_2}^{min}(3^2A)$	2.214	2.214	1.047	0.774	1.198	1.198	-180.00	2.180
H[d] (1)	2.217	2.217	1.045	0.773	1.203	1.203	180.00	2.183
H[d] (2)	2.234	2.215	1.044	0.773	1.206	1.213	180.00	2.190
H[d] (3)	2.215	2.234	1.044	0.773	1.213	1.206	180.00	2.190
Ref. 3	2.209	2.209	1.059	0.778			0.000	2.174

Table SI4. Entrance channel: Energies (cm^{-1}) and vibrational frequencies (cm^{-1}). First line for each species is the *ab initio* results.

	v_1	v_2	v_3	v_4	v_5	v_6	E
$Q_{OH+H_2}^{min}(1^2A)$	4408	3823					-33468
H[d] (1)	4410	3817					-33399
H[d] (2)	4406	3824					-33428
H[d] (3)	4406	3824					-33428
Ref. [1]	4401	3738					
$Q_{OH+H_2}^{min}(3^2A)$	4407	3303					0
H[d] (1)	4423	3294					0
H[d] (2)	4410	3303					-10
H[d] (3)	4410	3303					-10
Ref. 2	4382	3228					
$Q_{OH-H_2}^{min}(1^2A)$	4394	3825	345	135	110	105	-33620
H[d] (1)	4383	3821	367	223	168	54	-33631
H[d] (2)	4397	3817	407	222	143	122	-33630
H[d] (3)	4397	3817	407	222	143	122	-33630
Ref([3])							-33559
$Q_{OH-H_2}^{min}(3^2A)$	4015	2796	1431	758	755	482	-2793
H[d] (1)	3993	2827	1412	292	754	456	-2774
H[d] (2)	3986	2817	1404	747	694	477	-2759
H[d] (3)	3986	2817	1404	747	694	477	-2759
Ref. 3							-2511

Table SI5. Valence region minimum energy conical intersections**.** Energies are in cm^{-1}. First line for each species is the *ab initio* results. Distances are in Å. Angles are in degrees. ||**g**|| and ||**h**|| are in atomic units.

	$R(OH^a)$	$R(OH^b)$	$R(OH^c)$	$R(H^aH^b)$	H^aOH^b	$H^1OH^2H^3$	E	$\|\|\mathbf{g}\|\|$	$\|\|\mathbf{h}\|\|$
$Q^{mex}_{HO-H_2}(2,3^2A)\ (C_{2v})$	1.517	1.518	0.974	0.846	32.38	180.00	-10317	0.12910	0.10335
H[d] (1)	1.517	1.517	0.974	0.847	32.42	180.00	-10331	0.12989	0.10240
H[d] (2)	1.517	1.517	0.974	0.846	32.38	180.00	-10347	0.12869	0.10281
H[d] (3)	1.517	1.517	0.974	0.846	32.38	180.00	-10347	0.12869	0.10281
Ref. 4	1.514	1.514	0.977	0.841	32.36	180.00	-10448	0.12907	0.1032
$Q^{mex}_{HO-H_2}(2,3^2A)(colinear)$	1.195	2.135	0.962	0.940	0.01	179.01	-15471	0.15553	0.07750
H[d] (1)	1.197	2.137	0.963	0.940	0.00	180.00	-15598	0.15144	0.00001
H[d] (2)	1.210	2.122	0.962	0.930	6.61	180.00	-15598	0.15409	0.02711
H[d] (3)	1.196	2.135	0.963	0.939	0.09	180.00	-15577	0.15552	0.00455
Ref. 4	1.187	2.131	0.962	0.944	0.00	0.00	-15321	0.15580	0.07848
$Q^{mex}_{HO-H_2}(1,2^2A)\ (C_{2v})$	1.503	1.503	0.974	0.855	33.04	-180.00	-10689	0.12192	0.10438
H[d] (1)	1.503	1.503	0.974	0.856	33.08	180.00	-10697	0.12270	0.10391
H[d] (2)	1.503	1.503	0.975	0.854	33.03	180.00	-10710	0.12265	0.10412
H[d] (3)	1.503	1.503	0.975	0.854	33.03	180.00	-10710	0.12265	0.10412

Table I6. Geometric parameters of 2^2A-3^2A crossing seam obtained for fixed $\angle OH^aH^b$ using *ab initio* and $\boldsymbol{H}^d(1)$. Bold values are constrained during optimization. Distances are in Å. Angles are in degrees. Energies are in wavenumbers relative to the OH(A)+H_2 asymptote. ||**g**|| and ||**h**|| are in atomic units.

	$R(OH^a)$	$R(OH^b)$	$R(OH^c)$	$R(H^aH^b)$	OH^aH^b	$H^aOH^bH^c$	E	||**g**||	||**h**||
1	1.509	1.527	0.974	0.847	**75.00**	180.00	-10321	0.12909	0.10329
	1.508	1.527	0.974	0.848	**75.00**	180.00	-10334	0.12986	0.10236
2	1.473	1.568	0.974	0.850	**80.00**	180.00	-10410	0.12930	0.10267
	1.473	1.568	0.974	0.852	**80.00**	180.00	-10418	0.13007	0.10204
3	1.441	1.610	0.974	0.856	**85.00**	180.00	-10604	0.12992	0.10166
	1.440	1.610	0.974	0.857	**85.00**	180.00	-10607	0.13071	0.10147
4	1.411	1.654	0.973	0.863	**90.00**	180.00	-10885	0.13095	0.10027
	1.410	1.654	0.973	0.864	**90.00**	180.00	-10886	0.13174	0.10071
5	1.384	1.698	0.972	0.871	**95.00**	180.00	-11232	0.13234	0.09859
	1.383	1.698	0.973	0.871	**95.00**	180.00	-11236	0.13310	0.09984
6	1.359	1.742	0.972	0.880	**100.00**	180.00	-11622	0.13404	0.09671
	1.358	1.741	0.972	0.879	**100.00**	180.00	-11634	0.13472	0.09893
7	1.336	1.785	0.971	0.888	**105.00**	180.00	-12035	0.13597	0.09473
	1.336	1.784	0.971	0.886	**105.00**	180.00	-12056	0.13655	0.09794
8	1.316	1.827	0.970	0.895	**110.00**	180.00	-12454	0.13803	0.09273
	1.315	1.825	0.970	0.893	**110.00**	180.00	-12481	0.13849	0.09673
9	1.297	1.867	0.969	0.902	**115.00**	180.00	-12864	0.14014	0.09077
	1.297	1.865	0.969	0.900	**115.00**	180.00	-12890	0.14048	0.09504
10	1.281	1.905	0.968	0.908	**120.00**	180.00	-13255	0.14224	0.08888
	1.280	1.903	0.968	0.907	**120.00**	180.00	-13272	0.14245	0.09261
11	1.266	1.940	0.967	0.914	**125.00**	180.00	-13619	0.14425	0.08709
	1.265	1.939	0.967	0.913	**125.00**	180.00	-13621	0.14433	0.08922
12	1.253	1.971	0.966	0.917	**130.00**	180.00	-13953	0.14615	0.08543
	1.252	1.972	0.966	0.918	**130.00**	180.00	-13938	0.14608	0.08475
13	1.241	2.003	0.965	0.923	**135.00**	180.00	-14252	0.14792	0.08392
	1.241	2.003	0.966	0.923	**135.00**	180.00	-14225	0.14768	0.07917
14	1.231	2.031	0.964	0.927	**140.00**	180.00	-14516	0.14958	0.08251
	1.231	2.031	0.965	0.928	**140.00**	180.00	-14484	0.14911	0.07255
15	1.223	2.056	0.964	0.931	**145.00**	180.00	-14745	0.15122	0.08128
	1.222	2.056	0.965	0.931	**145.00**	180.00	-14720	0.15038	0.06503
16	1.215	2.077	0.963	0.934	**150.00**	180.00	-14941	0.15280	0.08023
	1.215	2.077	0.964	0.934	**150.00**	180.00	-14934	0.15150	0.05677
17	1.209	2.094	0.963	0.936	**155.00**	180.00	-15106	0.15422	0.07935
	1.209	2.096	0.964	0.937	**155.00**	180.00	-15124	0.15246	0.04795
18	1.204	2.109	0.963	0.937	**160.00**	180.00	-15240	0.15536	0.07864
	1.205	2.111	0.964	0.938	**160.00**	180.00	-15289	0.15328	0.03873
19	1.200	2.120	0.963	0.938	**165.00**	180.00	-15418	0.15603	0.07810
	1.201	2.123	0.963	0.940	**165.00**	180.00	-15457	0.15393	0.02923
20	1.197	2.129	0.962	0.939	**170.00**	180.00	-15415	0.15609	0.07771
	1.199	2.130	0.963	0.940	**169.00**	180.00	-15507	0.15432	0.02150
21	1.195	2.133	0.962	0.940	**175.00**	180.00	-15458	0.15575	0.07748
	1.198	2.136	0.963	0.940	**174.00**	180.00	-15579	0.14923	0.01519

Table SI7. Geometric and conical parameters of the 2^2A-3^2A seam. Constrained values are in bold. Distances are in Å. Angles are in degrees. Energies are in wavenumbers relative to the OH(A)+H_2 asymptote. $\phi = 90 - \cos^{-1}\left[R(OH^c)\cdot\left(R(OH^a)\times R(OH^b)\right)/\left(\|R(OH^c)\|\cdot\|\left(R(OH^a)\times R(OH^b)\right)\|\right)\right]$. ||**g**|| and ||**h**|| are in atomic units.

	R(OH^a)	*R*(OH^b)	R(OH^c)	*R*(H^{a}H^b)	H^{a}OH^b	ϕ	E	||**g**||	||**h**||
1	1.534	1.534	0.972	0.891	33.77	**1.86**	-9974	0.11635	0.09322
2	1.533	1.533	0.975	0.896	34.01	**2.77**	-9692	0.10679	0.08654
3	1.531	1.531	0.978	0.905	34.36	**3.66**	-9309	0.09774	0.07995
4	1.530	1.530	0.981	0.915	34.81	**4.51**	-8839	0.09013	0.07420
5	1.530	1.530	0.985	0.929	35.33	**5.32**	-8301	0.08405	0.06945
6	1.530	1.530	0.989	0.944	35.92	**6.08**	-7709	0.07927	0.06560
7	1.531	1.531	0.993	0.961	36.56	**6.81**	-7079	0.07547	0.06250
8	1.536	1.536	1.000	0.999	37.95	**8.13**	-5750	0.06978	0.05788
9	1.544	1.544	1.005	1.042	39.44	**9.28**	-4392	0.06537	0.05457
10	1.556	1.556	1.009	1.090	41.01	**10.27**	-3066	0.06121	0.05192
11	1.572	1.572	1.011	1.142	42.62	**11.86**	-1813	0.05655	0.04950
12	1.591	1.591	1.011	1.199	44.29	**12.47**	-654	0.05084	0.04693
13	1.611	1.611	1.011	1.259	45.99	**12.99**	430	0.04382	0.04374
14	1.628	1.628	1.020	1.314	47.61	**13.45**	1518	0.03969	0.03652

Table SI8. Geometric and conical parameters of the 1^2A-2^2A seam. Constrained values are in bold. Distances are in Å. Angles are in degrees. Energies are in wavenumbers relative to the OH(A)+H_2 asymptote. ||g|| and ||h|| are in atomic units.

	$R(OH^a)$	$R(OH^b)$	$R(OH^c)$	$R(H^aH^b)$	H^aOH^b	$H^aOH^bH^c$	E	**||g||**	**||h||**
1	**1.429**	1.607	0.972	0.879	32.99	180.00	-10721.94	0.12968	0.10024
	1.429	1.644	0.971	0.876	32.18	180.00	-10719.00	0.13035	0.10036
2	**1.482**	1.564	0.973	0.856	32.50	180.00	-10380.07	0.12888	0.10256
	1.482	1.563	0.973	0.857	32.54	180.00	-10388.80	0.12962	0.10189
3	**1.535**	1.497	0.974	0.842	32.23	180.00	-10330.48	0.12942	0.10343
	1.535	1.497	0.974	0.844	32.28	180.00	-10343.30	0.13020	0.10253
4	**1.588**	1.442	0.975	0.834	31.49	180.00	-10519.55	0.13090	0.10299
	1.588	1.442	0.975	0.835	31.54	180.00	-10523.40	0.13178	0.10261
5	**1.640**	1.394	0.975	0.830	30.36	180.00	-10879.76	0.13300	0.10180
	1.640	1.393	0.975	0.829	30.36	180.00	-10883.10	0.13407	0.10256

SI9. Linking region saddle point structures. First line for each species is the *ab initio* results.

Distances are in Å. Angles are in degrees.

	R(OH^a)	R(OH^b)	R(OH^c)	R(H^{a}H^b)	H^{a}OH^b	H^{b}OH^c	H^{a}OH^{b}H^c
$Q_{OH-H_2}^{ts}(2^2A)$	1.885	1.885	0.968	1.667	52.48	90.65	52.48
H^d (1)	1.907	1.907	0.968	1.693	52.71	92.35	52.76
H^d (2)	1.884	1.888	0.968	1.668	52.49	90.89	52.49
H^d (3)	1.888	1.884	0.968	1.668	52.49	90.47	52.49
Ref. 5	1.887	1.887	0.971	1.675			
$Q_{OH-H_2}^{ts}(1^2A)$	2.146	1.348	0.967	0.822	6.61	96.43	-0.04
H^d (1)	2.145	1.346	0.967	0.823	6.55	96.75	0.00
H^d (2)	2.137	1.348	0.967	0.821	7.61	97.26	0.00
H^d (3)	2.145	1.346	0.967	0.823	6.60	96.50	0.00
Ref. 6		1.356	0.970	0.819		96.50	

Table SI10. Linking Region: Energy (cm^{-1}) and vibrational frequencies (cm^{-1}) for Linking Region saddle point structures. First line for each species is the *ab initio* results.

	v_1	v_2	v_3	v_4	v_5	v_6	E
$Q_{OH-H_2}^{ts}(2^2A)$	3807	681	678	616	314	3085i	1962
H^d (1)	3770	1050	676	368	263	2446i	1841
H^d (2)	3776	719	687	499	429	3149i	1946
H^d (3)	3776	719	687	499	429	3149i	1946
Ref. 5	3733	963	674	610	326	2973i	706
$Q_{OH-H_2}^{ts}(1^2A)$	3812	2586	1080	611	455	1221i	-31199
H^d (1)	3781	2548	955	709	473	1452i	-31192
H^d (2)	3843	2560	858	559	415	1258i	-31183
H^d (3)	3817	2611	1085	594	534	1290i	-31214
Ref. 6	3771	2622	1051	598	501	1192i	-31462

Table SI11. Rydberg region minimum and saddle point structures. First line for each species is the *ab initio* results. Distances are in Å. Angles are in degrees.

	$R(OH^a)$	$R(OH^b)$	$R(OH^c)$	$R(H^aH^b)$	H^aOH^b	H^bOH^c	$H^aOH^bH^c$
$Q_{OH_3}^{min}(1^2A)$	1.014	1.014	1.016	1.615	105.51	105.57	111.49
H^d (1)	1.016	1.016	1.015	1.617	105.46	105.67	111.64
Ref. 4	1.025	1.025	1.025	NR	NR	NR	NR
$Q_{OH_3}^{ts}(1^2A)$	1.009	1.009	1.009	1.748	120.00	120.00	180.00
H^d (1)	1.008	1.008	1.008	1.744	119.85	120.07	180.00
$Q_{H_2O-H}^{ts}(1^2A)$	0.985	0.985	1.213	1.562	104.95	103.82	109.52
H^d (1)	0.986	0.986	1.212	1.567	105.23	103.91	108.92
H^d (2)	0.986	0.985	1.210	1.562	104.55	104.27	109.85
H^d (3)	0.985	0.986	1.210	1.562	104.87	104.55	109.85
Ref. 4	0.988	0.988	1.225	1.562			
$Q_{OH_3}^{min}(4^2A)$	0.972	0.971	0.972	1.623	113.26	113.26	130.73
H^d (1)	0.971	0.971	0.971	1.618	112.93	113.37	130.68

Table SI12. Rydberg Region: Electronic energy (cm^{-1}) and vibrational frequencies (cm^{-1}). First line for each species is the *ab initio* results. Distances are in Å. Angles are in degrees.

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6	E
$Q_{OH_3}^{min}(1^2A)$	2998	2748	2597	1474	1426	979	-32433
H[d] (1)	2941	2525	2495	1480	1457	989	-32468
Ref. 4							-30742
$Q_{OH_3}^{ts}(1^2A)$	2890	2634	2633	1248	1248	787i	-30670
H[d] (1)	2843	2674	2605	1410	1328	669i	-30897
$Q_{H_2O-H}^{ts}(1^2A)$	3446	3380	1580	1016	817	1929i	-31396
H[d] (1)	3428	3309	1616	1079	825	1896i	-31483
H[d] (2)	3465	3404	1533	1103	893	1907i	-31477
H[d] (3)	3465	3404	1533	1103	893	1907i	-31477
Ref. 4							-29532
$Q_{OH_3}^{min}(4^2A)$	3849	3849	3675	1697	1696	817	-9179
H[d] (1)	3807	3782	3689	1712	1693	771	-9182

Table SI13. Rydberg region conical intersection structures, energies (cm^{-1}), and conical parameters (a.u.). No *ab initio* determined results for these structures. Distances are in Å. Angles are in degrees. ||**g**|| and ||**h**|| are in atomic units.

	$R(OH^a)$	$R(OH^b)$	$R(OH^c)$	$R(H^aH^b)$	H^aOH^b	H^bOH^c	$H^aOH^bH^c$	E	$\|\|\mathbf{g}\|\|$	$\|\|\mathbf{h}\|\|$
$Q_{OH_3}^{mex}(2,3^2A)\ (C_{3v})$ **H^d (1)**	0.988	0.988	0.989	1.633	111.52	111.51	125.37	-14378	0.02919	0.02909
Ref. 7	0.987	0.987	0.987	1.620				-12519	0.03107	0.03107
$Q_{OH_3}^{mex}(2,3^2A)\ (D_{3h})$ **H^d (1)**	0.975	0.975	0.989	1.672	118.08	120.96	180.00	-13493	0.02329	0.00000
Ref. 7	0.973	0.973	0.973	1.686				-11638	0.02451	0.02451

Table SI14. Product channel: structures, vibrational frequencies, and energies. Distances are in Å. Angles are in degrees. Energies are in cm^{-1}.

	$R(OH^a)$	$R(OH^b)$	H^aOH^b	ν_1	ν_2	ν_3	E
$Q_{H_2O+H}^{min}(1^2A)$	0.958	0.958	104.07	3975	3875	1674	-39010
H^d (1)	0.957	0.957	103.77	3951	3841	1714	-38989
H^d (2)	0.957	0.957	104.20	3978	3912	1700	-39036
H^d (3)	0.957	0.957	104.20	3978	3912	1700	-39036
Ref . 5	0.958	0.958		3912	3831	1669	-38989
Ref . 8	0.959	0.959	104.30	3936	3825	1654	

Table SI15. Geometric parameters for Jahn-Teller minima and saddle points for Rydberg region 2^2A-3^2A C_{3v} MEX. Distances are in Å. Angles are in degrees.

	$R(OH^a)$	$R(OH^b)$	$R(OH^c)$	$R(H^aH^b)$	$R(H^aH^c)$	$R(H^bH^c)$	H^aOH^b	H^aOH^c	H^bOH^c	$H^aOH^bH^c$
$Q_{OH_3}^{JT,min}(2^2A)$	0.978	0.978	1.019	1.578	1.659	1.659	107.55	112.35	112.35	124.14
$Q_{OH_3}^{JT,min}(2^2A)$	1.019	0.976	0.981	1.657	1.577	1.670	112.24	113.20	107.34	124.99
$Q_{OH_3}^{JT,min}(2^2A)$	0.976	1.019	0.981	1.657	1.670	1.577	112.24	107.34	113.20	124.99
$Q_{OH_3}^{JT,ts}(2^2A)$	1.003	1.003	0.969	1.677	1.610	1.610	113.45	109.51	109.51	122.67
$Q_{OH_3}^{JT,ts}(2^2A)$	0.969	0.999	1.009	1.596	1.680	1.622	108.72	110.10	113.95	122.45
$Q_{OH_3}^{JT,ts}(2^2A)$	0.995	0.969	1.009	1.596	1.622	1.680	108.72	113.95	110.10	122.45

Table SI16. Vibrational frequencies (cm^{-1}) and coordinates (a.u.) in **g-h** plane for Jahn-Teller minima and saddle points for Rydberg region 2^2A-3^2A C_{3v} MEX. Energies (cm^{-1}) are relative to the 2^2A-3^2A C_{3v} MEX. x and y represent coordinates in the **g-h** plane (in atomic units), where $x = \mathbf{g}/||\mathbf{g}||$ and $y = \mathbf{h}/||\mathbf{h}||$.

	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6	E	x	y
$Q_{OH_3}^{JT,min}(2^2A)$	3597	2698	2504	1606	859	788	-201	0.00196	0.00000
$Q_{OH_3}^{JT,min}(2^2A)$	3632	2771	2581	1657	1280	846	-237	-0.00089	-0.00199
$Q_{OH_3}^{JT,min}(2^2A)$	3632	2771	2581	1657	1280	846	-237	-0.00089	0.00199
$Q_{OH_3}^{JT,ts}(2^2A)$	3757	2961	2197	1693	811	1614*i*	-189	-0.00165	0.00000
$Q_{OH_3}^{JT,ts}(2^2A)$	3747	2899	2207	1579	879	1080*i*	-193	0.00136	0.00121
$Q_{OH_3}^{JT,ts}(2^2A)$	3747	2899	2207	1579	879	1080*i*	-193	0.00135	-0.00118

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