

## Supporting Information

Seams of Conical Intersections Relevant to the Quenching of  $\text{OH}(A^2\Sigma^+)$  by Collisions with

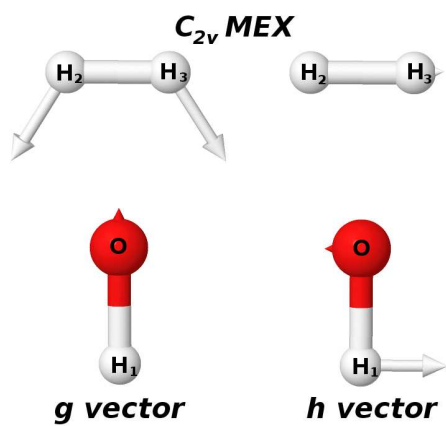
$\text{H}_2$ .

Joseph Dillon and David R. Yarkony

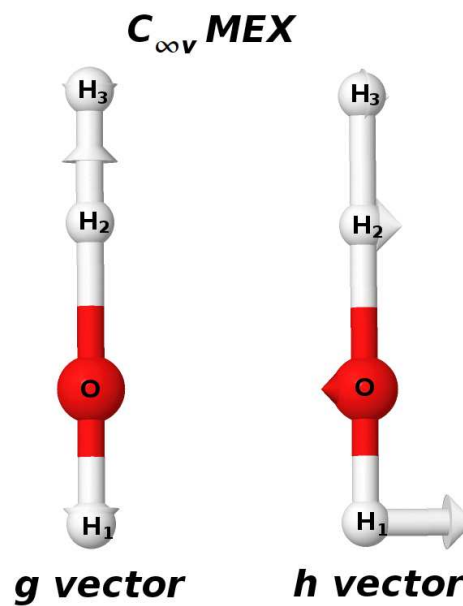
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**g** and **h** for references geometries

(S1a)

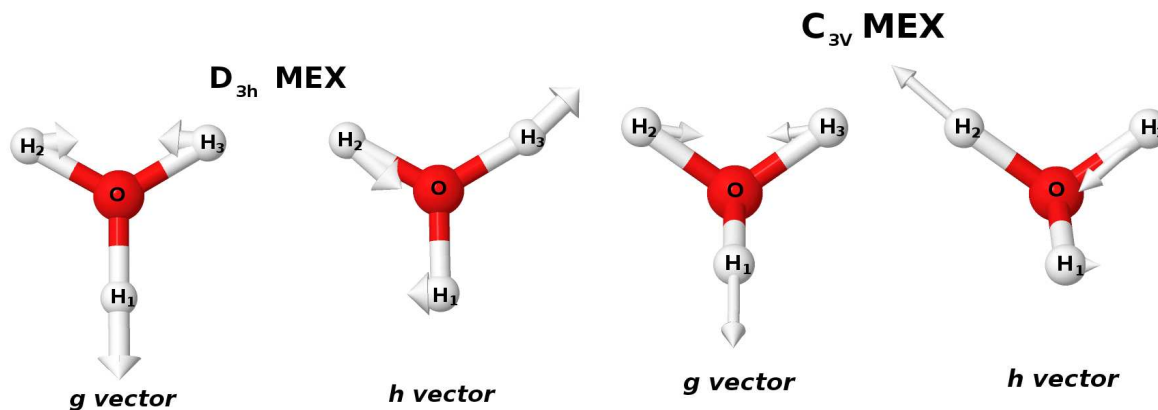


(S1b)



(S1c)

(S1d)



## Section I-Internal Coordinates, Energies and Conical Parameters for the EMIs

Important internal coordinates ( $R(\text{OH}^1)$ ,  $R(\text{OH}^2)$ ,  $R(\text{OH}^3)$ ,  $R(\text{H}^2\text{H}^3)$ ,  $\theta_1$ ,  $\theta_2$ , and  $\varphi$ ), conical parameters  $g$ ,  $h$ ,  $s_x$  and  $s_y$  and energies for all the *EMI* presented in the work are tabulated below. The sets of intersections are grouped as follows:

Presented in Tables SIa-d are the planar intersections reported in this work. The constrained MEX points, as functions of  $R(\text{OH}^2)$ ,  $R(\text{OH}^3)$ , can be pictured as displacements in the  $\theta_2$  coordinate originating from the high symmetry  $C_{2v}$  (Tables SIa-b) and  $C_{\infty v}$  (Tables SIc-d) intersections, yielding points of MEX that have only  $C_s$  planar symmetry. For each of these constraints,  $R(\text{OH}^2)$  and  $R(\text{OH}^3)$ , both  $1^2A''-1^2A'$  (Tables SIb and SIc) and  $1,2^2A'$  (Tables SIa and SIc) seam points were optimized.

Presented in Tables SIIa-SIIg (Tables SIIIa-SIIIk) are the extension of the  $1,2^2A'$  seam points presented in Tables SIa(SIc) to nonplanar geometries. These intersections have three geometric constraints, the same  $R(\text{OH}^2)$ ,  $R(\text{OH}^3)$  as in the planar MEXs in addition to the  $\varphi$  coordinate. Thus, Tables SIIa-SIIg(SIIIa-SIIIk) tabulate extensions of the near-

$Q_{2,3}^{mex}(C_{2v})$  (near- $Q_{2,3}^{mex}(C_{3v})$ ) planar intersection points to out-of-plane regions where the molecule has no point group symmetry and the intersections involve the  $2,3^2A$  electronic states.

Presented in Tables SIVa-SIVb are different portions of the  $1,2^2A'$  seam of conical intersection for nonplanar geometries. Here, these intersections have only two geometric constraints, the  $R(H^2H^3)$  bond distance and the  $\varphi$  coordinate. For Tables SIVa, the  $R(H^2H^3)$  bond distance is about equal to the entrance channel  $R(H^2H^3)$  bond distance and for Tables SIVb, the  $R(H^2H^3)$  bond distance is set to be equal to  $R(H^2H^3)$  bond distance at the  $C_{2v}$  MEX point.

Presented in Tables SVa are extensions of the  $D_{3h}$  MEX point, portions of the  $2,3^2A'$  seam of conical intersection, to nonplanar geometries of  $C_{3v}$  point group symmetry. These are symmetry required degeneracies,  $1^2E'$ , and result from the Rydberg character of the electronic structure in this region. Along this path, these intersections have no geometric constraints, and are just displacements in the  $\varphi$  coordinate for which the degeneracy of the intersections must persist based on symmetry arguments.

**Table S1a-**

Points on  $1^2A'$ - $2^2A'$  seam of conical intersection as deviations in  $R(\text{OH}^2)$  and  $R(\text{OH}^3)$ , from  $\mathbf{Q}_{2,3}^{max}(C_{2v})$ ,  $\phi=0$ .

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	1	2	3	4	5	6	7
$R(\text{OH}^1)$	1.8476	1.8507	1.8512	1.8522	1.8539	1.8562	1.8567
$R(\text{OH}^2)$	2.8629	2.8000	2.7000	2.6000	2.5000	2.4000	2.3000
$R(\text{OH}^3)$	2.8629	2.9000	3.0000	3.1000	3.2000	3.3000	3.4000
$R(\text{H}^2\text{H}^3)$	1.5907	1.5612	1.5521	1.5341	1.5098	1.4812	1.4653
$R_x$	2.7502	2.7415	2.7464	2.7562	2.7704	2.7886	2.8066
$\theta_1$	180	180	180	180	180	180	180
$\theta_2$	90	86	78	70	62	52	40
$E_1$	-12445	-12417	-12530	-12716	-12901	-12989	-12714
$E_2$	-10448	-10450	-10627	-10940	-11317	-11666	-11963
$E_3$	-10448	-10450	-10627	-10940	-11317	-11666	-11963
$  g  $	.129073	.13003	.13124	.13361	.13701	.14127	.14799
$  h  $	.103197	.10374	.10312	.10197	.10026	.09795	.09502
$s_x$	.00914	.00927	.00897	.00836	.00744	.00624	.00514
$s_y$	0	0.00009	.00029	.00056	.00089	.00122	.00158

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**Table S1b-**

Points on  $1^2A' - 1^2A''$  seam of conical intersection as deviations, in  $R(OH^2)$  and  $R(OH^3)$  from  $Q_{2,3}^{max}(C_{2v})$ ,  $\phi=0$ .

	1	2	3	4	5	6	7
$R(OH^1)$	1.8841	1.8915	1.8831	1.8821	1.8807	1.8787	1.8769
$R(OH^2)$	2.8500	2.8000	2.7000	2.6000	2.5000	2.4000	2.3000
$R(OH^3)$	2.8500	2.9000	3.0000	3.1000	3.2000	3.3000	3.4000
$R(H^2H^3)$	1.3604	1.3603	1.3612	1.3636	1.3677	1.3747	1.3809
$R_x$	2.7677	2.7681	2.7714	2.7786	2.7888	2.8022	2.8193
$\theta_1$	171	172	172	173	174	175	176
$\theta_2$	90	86	77	68	58	48	36
$E_1$	-13851	-13821	-13745	-13643	-13496	-13278	-12946
$E_2$	-13851	-13821	-13745	-13643	-13496	-13278	-12946
$E_3$	-6275	-6279	-6454	-6853	-7483	-8326	-9362
$  g  $	0.0446	0.0447	0.04513	0.04576	0.04666	0.04794	0.05001
$  h  $	0.0453	0.0456	0.04623	0.04690	0.04764	0.04851	0.04977
$s_x$	0.0017	0.0018	0.00188	0.00203	0.00226	0.00258	0.00307
$s_y$	0.0	0.0	0.0	0.0	0.0	0.0	0.0

**Table SIc -**

Points on  $1^2A'$ -  $2^2A'$  seam of conical intersection as deviations, in  $R(OH^2)$  and  $R(OH^3)$  from  $Q_{2,3}^{max}(C_{xy})$ ,  $\phi=0$ .

	1	2	3	4	5	6	7	8	9	10	11
$R(OH^1)$	1.8099	1.8093	1.8092	1.8092	1.8094	1.8098	1.8103	1.8111	1.8121	1.8132	1.8132
$R(OH^2)$	2.2500	2.3000	2.3500	2.4000	2.4500	2.5000	2.5500	2.600	2.6500	2.7000	2.7500
$R(OH^3)$	4.0000	3.9500	3.9000	3.8500	3.8000	3.7500	3.7000	3.6500	3.6000	3.5500	3.5000
$R(H^2H^3)$	1.7749	1.8070	1.8405	1.8750	1.9102	1.9457	1.9812	2.0165	2.0510	2.0843	2.1159
$R_x$	3.1215	3.1032	3.0854	3.0680	3.0511	3.0348	3.0191	3.0041	2.9899	2.9766	2.9643
$\theta_1$	180	179	178	178	178	178	178	178	178	178	178
$\theta_2$	9	23	31	38	44	49	53	57	61	65	68
$E_1$	-15264	-14943	-14525	-14026	-13463	-12854	-12213	-11556	-10900	-10258	-9646
$E_2$	-15220	-14681	-14065	-13385	-12657	-11894	-11113	-10327	-9552	-8802	-8093
$E_3$	-15220	-14681	-14065	-13385	-12657	-11894	-11113	-10327	-9552	-8802	-8093
$  g  $	.15558	.15208	.14859	.14514	.14175	.13842	.13516	.13197	.12885	.12582	.12289
$  h  $	.07938	.08061	.08170	.08266	.08346	.08410	.08458	.08492	.08513	.08521	.08520
$s_x$	.00332	.00311	.00301	.00299	.00301	.00305	.00310	.00315	.00321	.00326	.00332
$s_y$	.00021	.00039	.00037	.00031	.00024	.00017	.00013	.00010	.00009	.00010	.00013

**Table SId -**

Points on  $1^2A'$ -  $1^2A''$  seam of conical intersection as deviations in  $R(OH^2)$ ,  $R(OH^3)$  from  $Q_{2,3}^{max}(C_{ov})$ ,  $\phi=0$ .

	1	2	3	4	5	6	7	8	9	10	11
$R(OH^1)$	1.8616	1.8597	1.8580	1.8564	1.8562	1.8569	1.8575	1.8583	1.8587	1.8589	1.8592
$R(OH^2)$	2.2500	2.3000	2.3500	2.4000	2.4500	2.5000	2.5500	2.6000	2.6500	2.7000	2.7500
$R(OH^3)$	4.0000	3.9500	3.9000	3.8500	3.8000	3.7500	3.7000	3.6500	3.6000	3.5500	3.5000
$R(H^2H^3)$	1.7500	1.6500	1.5501	1.4505	1.3948	1.3844	1.3803	1.3735	1.3714	1.3696	1.3681
$R_x$	3.1250	3.1250	3.1250	3.1249	3.1200	3.1108	3.1016	3.0935	3.0856	3.0785	3.0722
$\theta_1$	180	180	180	179	175	172	170	166	165	165	165
$\theta_2$	0	0	1	2	14	25	33	39	45	51	56
$E_1$	-15820	-17633	-14065	-20162	-20600	-20845	-21109	-21282	-21364	-21420	-21456
$E_2$	-15820	-17633	-14065	-20162	-20600	-20845	-21109	-21282	-21364	-21420	-21456
$E_3$	-14764	-13237	-11562	-9642	-8231	-7629	-7148	-6528	-6138	-5789	-5480
$  g  $	.0000	.0000	.0003	.0006	.0053	.0087	.0108	.0169	.0175	.0174	.0184
$  h  $	.0000	.0000	.0003	.0006	.0053	.0086	.0107	.0146	.0158	.0167	.0176
$s_x$	.0000	.0000	.0000	.0000	.0000	.0000	.0001	.0003	.0003	.0003	.0003
$s_y$	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000

**Table SIIa -**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.8629=R(\text{OH}^3)$  at  $C_{2v}$  MEX to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6	7	8
$\varphi$	2.5	5.0	7.5	10.0	12.5	15.0	17.5	20.0
R(OH <sup>1</sup> )	1.8475	1.8485	1.8516	1.8593	1.8683	1.8779	1.8897	1.9094
R(OH <sup>2</sup> )	2.8629	2.8629	2.8629	2.8629	2.8629	2.8629	2.8629	2.8629
R(OH <sup>3</sup> )	2.8629	2.8629	2.8629	2.8629	2.8629	2.8629	2.8629	2.8629
R(H <sup>2</sup> H <sup>3</sup> )	1.6095	1.6620	1.7405	1.8977	2.0077	2.1227	2.2441	2.3827
R <sub>x</sub>	2.7475	2.7397	2.7275	2.7011	2.6812	2.6589	2.6339	2.6033
$\theta_1$	180	180	180	180	180	180	180	180
$\theta_2$	90	90	90	90	90	90	90	90
E <sub>1</sub>	-12556	-12809	-13047	-12529	-12482	-12357	-12171	-11864
E <sub>2</sub>	-10123	-9150	-7564	-4687	-2212	-378	3016	5782
E <sub>3</sub>	-10123	-9150	-7564	-4687	-2212	-378	3016	5782
g	.11616	.09518	.07993	.06728	.06217	.05855	.05521	.05057
h	.09448	.07926	.06717	.05532	.05011	.04616	.04276	.03939
s <sub>x</sub>	.00854	.00721	.00605	.00526	.00489	.00455	.00411	.00325
s <sub>y</sub>	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000



**Table SIIf -**

Extension of 1,2 A' constrained R(OH<sup>2</sup>)=2.80 R(OH<sup>3</sup>)=2.90 planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6	7	8
$\Phi$	2.5	5.0	7.5	10.0	12.5	15.0	17.5	20.0
R(OH <sup>1</sup> )	1.8508	1.8513	1.8536	1.8609	1.8704	1.8805	1.8901	1.9093
R(OH <sup>2</sup> )	2.8000	2.8000	2.8000	2.8000	2.8000	2.8000	2.8000	2.8000
R(OH <sup>3</sup> )	2.9000	2.9000	2.9000	2.9000	2.9000	2.9000	2.9000	2.9000
R(H <sup>2</sup> H <sup>3</sup> )	1.5802	1.6334	1.7126	1.8690	1.9794	2.0944	2.2147	2.3501
R <sub>x</sub>	2.7388	2.7309	2.7188	2.6929	2.6731	2.6511	2.6265	2.5970
$\theta_1$	180	180	180	180	180	179	179	179
$\theta_2$	86	86	86	87	87	87	87	87
E <sub>1</sub>	-12556	-12874	-13185	-12766	-12758	-12658	-12500	-12215
E <sub>2</sub>	-10142	-9207	-7658	-4827	-2357	238	2886	5644
E <sub>3</sub>	-10142	-9207	-7658	-4827	-2357	238	2886	5644
g	0.11653	0.0950	0.07971	.06716	.06221	.05878	.05565	.05147
h	0.09470	.07918	0.0671	.05533	.05024	.04640	.04314	.03996
s <sub>x</sub>	0.00865	.00732	.00617	.00538	.00503	.00473	.00430	.00353
s <sub>y</sub>	0.	0.0	0.0	0.0	0.0	0.0	0.0	0.

**Table IIIc-**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.70$   $R(\text{OH}^3)=3.00$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6	7	8
$\varphi$	2.5	5.0	7.5	10.0	12.5	15.0	17.5	20.0
R(OH <sup>1</sup> )	1.8484	1.8494	1.8533	1.8612	1.8700	1.8788	1.8889	1.9092
R(OH <sup>2</sup> )	2.7000	2.7000	2.7000	2.7000	2.7000	2.7000	2.7000	2.7000
R(OH <sup>3</sup> )	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000	3.0000
R(H <sup>2</sup> H <sup>3</sup> )	1.6064	1.6679	1.7559	1.8593	1.9704	2.0866	2.2092	2.3491
R <sub>x</sub>	2.7386	2.7294	2.7155	2.6983	2.6785	2.6564	2.6315	2.6010
$\theta_1$	180	180	180	179	179	178	177	176
$\theta_2$	79	79	80	80	81	81	82	82
E <sub>1</sub>	-12245	-12596	-12915	-13091	-13126	-13059	-12913	-12608
E <sub>2</sub>	-10083	-9001	-7281	-5092	-2617	-1	-2697	-5553
E <sub>3</sub>	-10083	-9001	-7281	-5092	-2617	-1	-2697	-5553
g	.11369	.08888	.07408	.06588	.06101	.05764	.05462	.05052
h	.09103	.07342	.06163	.05430	.04940	.04576	.04273	.03992
s <sub>x</sub>	.00832	.00686	.00585	.00532	.00498	.00468	.00430	.00360
s <sub>y</sub>	.00030	.00016	.00005	.00004	.00013	.00022	.00034	.00057

**Table SII d-**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.60$   $R(\text{OH}^3)=3.10$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6	7	8
$\varphi$	2.5	5	7.5	10	12.5	15	17.5	20
R(OH <sup>1</sup> )	1.8520	1.8519	1.8533	1.8594	1.8677	1.8766	1.8870	1.9098
R(OH <sup>2</sup> )	2.6000	2.6000	2.6000	2.6000	2.6000	2.6000	2.6000	2.6000
R(OH <sup>3</sup> )	3.1000	3.1000	3.1000	3.1000	3.1000	3.1000	3.1000	3.1000
R(H <sup>2</sup> H <sup>3</sup> )	1.5537	1.6084	1.6903	1.8421	1.9553	2.0745	2.2020	2.3524
R <sub>x</sub>	2.7535	2.7456	2.7333	2.7086	2.6887	2.6663	2.6406	2.6080
$\theta_1$	180	180	180	179	178	177	175	173
$\theta_2$	71	71	72	73	74	75	76	77
E <sub>1</sub>	-12905	-13351	-13825	-13700	-13818	-13810	-13694	-13352
E <sub>2</sub>	-10655	-9775	-8276	-5552	-3063	-395	2401	-5471
E <sub>3</sub>	-10655	-9775	-8276	-5552	-3063	-395	2401	-5471
g	.11663	.09177	.07511	.06320	.05852	.05533	.05249	.04851
h	.09174	.07530	.06318	.05221	.04770	.04443	.04178	.03949
s <sub>x</sub>	.00802	.00687	.00567	.00514	.00483	.00456	.00423	.00364
s <sub>y</sub>	.00042	.00019	.0.0000	.00003	.00016	.00029	.00045	.00072

**Table IIIe -**

Extension of 1,2 A' constrained  $R(OH^2)=2.50$   $R(OH^3)=3.20$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6	7	8
$\Phi$	2.5	5	7.5	10	12.5	15	17.5	20
$R(OH^1)$	1.8533	1.8527	1.8529	1.8582	1.8668	1.8758	1.8880	1.9160
$R(OH^2)$	2.5000	2.5000	2.5000	2.5000	2.5000	2.5000	2.5000	2.5000
$R(OH^3)$	3.2000	3.2000	3.2000	3.2000	3.2000	3.2000	3.2000	3.2000
$R(H^2H^3)$	1.5304	1.5872	1.6742	1.8229	1.9399	2.0644	2.2006	2.3728
$R_x$	2.7676	2.7596	2.7467	2.7229	2.7026	2.6795	2.6522	2.6149
$\theta_1$	180	180	179	178	177	176	174	171
$\theta_2$	62	63	64	66	68	69	70	71
$E_1$	-13147	-13732	-14381	-14514	-14751	-14830	-14752	-14330
$E_2$	-11052	-10215	-8744	-6081	-3560	-806	2159	5644
$E_3$	-11052	-10215	-8744	-6081	-3560	-806	2159	5644
$\ g\ $	.11560	.08739	.06752	.05893	.05467	.05180	.04920	.04524
$\ h\ $	.08850	.07112	.05916	.04897	.04507	.04232	.04016	.03832
$s_x$	.00744	.00641	.00442	.00484	.00457	.00434	.00405	.00354
$s_y$	.00067	.00033	.00009	.00003	.00014	.00029	.00046	.00066

**Table SII f-**

Extension of 1,2 A' constrained R(OH<sup>2</sup>)=2.40 R(OH<sup>3</sup>)=3.30 planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6	7	8
$\varphi$	2.5	5	7.5	10	12.5	15	17.5	20
R(OH <sup>1</sup> )	1.8553	1.8532	1.8534	1.8589	1.8675	1.8775	1.8843	1.9773
R(OH <sup>2</sup> )	2.4000	2.4000	2.4000	2.4000	2.4000	2.4000	2.4000	2.4000
R(OH <sup>3</sup> )	3.2000	3.2000	3.2000	3.2000	3.2000	3.2000	3.2000	3.2000
R(H <sup>2</sup> H <sup>3</sup> )	1.5037	1.5661	1.6960	1.8089	1.9318	2.0649	2.2430	2.4481
R <sub>x</sub>	2.7856	2.7770	2.7579	2.7399	2.7188	2.6943	2.6967	2.6128
$\theta_1$	180	180	179	178	176	172	171	166
$\theta_2$	52	54	57	59	61	63	64	66
E <sub>1</sub>	-13325	-14124	-14841	-15465	-15853	-15629	-14752	-14791
E <sub>2</sub>	-11423	-10618	-8713	-6515	-3924	-1027	1588	6901
E <sub>3</sub>	-11423	-10618	-8713	-6515	-3924	-1027	1588	6901
g	.11169	.07896	.05927	.05293	.04946	.04711	.04390	.04029
h	.08330	.06453	.04957	.04451	.04148	.03943	.03714	.03614
s <sub>x</sub>	.00679	.00571	.00477	.00440	.00419	.00398	.00348	.00322
s <sub>y</sub>	.00089	.000436	.00033	.00011	.00007	.00024	.00037	.00030

**Table SII g-**

Extension of 1,2 A' constrained  $R(OH^2)=2.30$   $R(OH^3)=3.40$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6	7
$\varphi$	2.5	5	7.5	10	12.5	15	17.5
$R(OH^1)$	1.8553	1.8534	1.8562	1.8636	1.8717	1.8826	1.9013
$R(OH^2)$	2.5000	2.5000	2.5000	2.5000	2.5000	2.5000	2.5000
$R(OH^3)$	3.2000	3.2000	3.2000	3.2000	3.2000	3.2000	3.2000
$R(H^2H^3)$	1.4993	1.5820	1.6891	1.8096	1.9414	2.0884	2.2706
$R_x$	2.8041	2.7927	2.7770	2.7580	2.7355	2.7083	2.6713
$\theta_1$	177.5	175	172.5	170	166.5	163.2	159.2
$\theta_2$	41.8	44.8	48.1	51.1	53.8	56.3	58.9
$E_1$	-13328	-14552	-15685	-16522	-17080	-17383	-17371
$E_2$	-11644	-10619	-8905	-6631	-3911	-778	3016
$E_3$	-11644	-10619	-8905	-6631	-3911	-778	3016
$  g  $	.08864	.05912	.04940	.04529	.04309	.04151	.03951
$  h  $	.06700	.04906	.04211	.03887	.03706	.03587	.03485
$s_x$	.00609	.00459	.00401	.00380	.00366	.00348	.00319
$s_y$	.00104	.00063	.00039	.00019	.00002	.00014	.00024

**Table SIII a -**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.75$   $R(\text{OH}^3)=3.50$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

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	1	2	3	4	5	6
$\Phi$	2.5	5	7.5	10	12.5	15
$R(\text{OH}^1)$	1.8163	1.8213	1.8280	1.8375	1.8482	1.8682
$R(\text{OH}^2)$	2.7500	2.7500	2.7500	2.7500	2.7500	2.7500
$R(\text{OH}^3)$	3.5000	3.5000	3.5000	3.5000	3.5000	3.5000
$R(\text{H}^2\text{H}^3)$	2.1355	2.1915	2.2771	2.3873	2.5230	2.8835
$R_x$	2.9608	2.9505	2.9343	2.9123	2.8835	2.8396
$\theta_1$	178	177	176	175	173	170
$\theta_2$	68	69	69	70	71	72
$E_1$	-9613	-9510	-9342	-9106	-8788	-8208
$E_2$	-7667	-6458	-4633	-2361	269	3548
$E_3$	-7667	-6458	-4633	-2361	269	3548
$\ g\ $	.10684	.08252	.06595	.05541	.04775	.03982
$\ h\ $	.07667	.06234	.05134	.04373	.03815	.03321
$s_x$	0.00376	.00369	.00321	.00277	.00237	.00190
$s_y$	.00005	.00009	.00021	.00030	.00037	.00042

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**Table SIII b -**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.70$   $R(\text{OH}^3)=3.55$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6
$\varphi$	2.5	5	7.5	10	12.5	15
$R(\text{OH}^1)$	1.8150	1.8201	1.8267	1.8363	1.8473	1.8694
$R(\text{OH}^2)$	2.7000	2.7000	2.7000	2.7000	2.7000	2.7000
$R(\text{OH}^3)$	3.5500	3.5500	3.5500	3.5500	3.5500	3.5500
$R(\text{H}^2\text{H}^3)$	2.1043	2.1622	2.2506	2.3650	2.5070	2.7172
$R_x$	2.9732	2.9628	2.9463	2.9238	2.8940	2.8462
$\theta_1$	177	177	176	174	172	168
$\theta_2$	65	66	66	67	69	70
$E_1$	-10238	-10151	-9998	-9768	-9440	-8777
$E_2$	-8368	-7112	-5211	-2839	-40	3591
$E_3$	-8368	-7112	-5211	-2830	-40	3591
$\ g\ $	.10726	.08085	.06392	.05344	.04616	.03835
$\ h\ $	.07580	.06079	.04982	.04268	.03715	.03228
$s_x$	.00386	.00381	.00327	.002812	.00241	.00194
$s_y$	.00003	.00011	.00023	.00032	.00038	.00039



**Tablel SIII c -**

Extension of 1,2 A' constrained  $R(OH^2)=2.65$   $R(OH^3)=3.60$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

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	1	2	3	4	5	6
$\Phi$	2.5	5	7.5	10	12.5	15
$R(OH^1)$	1.8140	1.8190	1.8276	1.8355	1.8469	1.8749
$R(OH^2)$	2.6500	2.6500	2.6500	2.6500	2.6500	2.6500
$R(OH^3)$	3.6000	3.6000	3.6000	3.6000	3.6000	3.6000
$R(H^2H^3)$	2.0722	2.1325	2.2246	2.3435	2.4929	2.7289
$R_x$	2.9863	2.9756	2.9587	2.9357	2.9048	2.8512
$\theta_1$	177	177	176	174	171	167
$\theta_2$	61	62	63	64	66	68
$E_1$	-10882	-10817	-10685	-10472	-10140	-9353
$E_2$	-9091	-7782	-5795	-3294	-324	3783
$E_3$	-9091	-7782	-5795	-3294	-324	3783
$\ g\ $	.10756	.07847	.06136	.05129	.04425	.03646
$\ h\ $	.07462	.05887	.04800	.04097	.03596	.03109
$s_x$	.00402	.00392	.00333	.00280	.00242	.00196
$s_y$	.00001	.00001	.00024	.00032	.00038	.00032

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**Table SIII d -**

Extension of 1,2 A' constrained R(OH<sup>2</sup>)=2.60 R(OH<sup>3</sup>)=3.65 planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6
$\varphi$	2.5	5	7.5	10	12.5	15
R(OH <sup>1</sup> )	1.8130	1.8183	1.8262	1.8351	1.8480	1.9019
R(OH <sup>2</sup> )	2.6000	2.6000	2.6000	2.6000	2.6000	2.6000
R(OH <sup>3</sup> )	3.6500	3.6500	3.6500	3.6500	3.6500	3.6500
R(H <sup>2</sup> H <sup>3</sup> )	2.0391	2.1024	2.1988	2.3235	2.4819	2.7682
R <sub>x</sub>	3.0002	2.9893	2.9719	2.9481	2.9156	2.8505
$\theta_1$	177	177	175	173	171	165
$\theta_2$	58	59	60	61	63	65
E <sub>1</sub>	-11546	-11511	-11411	-11221	-10891	-9740
E <sub>2</sub>	-9837	-8463	-6377	-3738	-559	4419
E <sub>3</sub>	-9837	-8463	-6377	-3738	-559	4419
g	.10598	.07518	.05820	.04861	.04199	.03385
h	.07297	.05646	.04583	.03921	.03455	.02937
s <sub>x</sub>	.00421	.00401	.00334	.00282	.00240	.00195
s <sub>y</sub>	.00002	.00012	.00023	.00032	.00036	.00018

**Table SIII e -**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.55$   $R(\text{OH}^3)=3.70$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6
$\varphi$	2.5	5	7.5	10	12.5	15
R(OH <sup>1</sup> )	1.8123	1.8179	1.8261	1.8352	1.8481	1.8243
R(OH <sup>2</sup> )	2.5500	2.5500	2.5500	2.5500	2.5500	2.5500
R(OH <sup>3</sup> )	3.7000	3.7000	3.7000	3.7000	3.7000	3.7000
R(H <sup>2</sup> H <sup>3</sup> )	2.0052	2.0725	2.1744	2.3059	2.4761	2.9131
R <sub>x</sub>	3.0151	3.0037	2.9857	2.9609	2.9264	2.8240
$\theta_1$	177	177	175	173	170	160
$\theta_2$	54	55	56	58	60	64
E <sub>1</sub>	-12225	-12230	-12173	-12017	-11694	-10605
E <sub>2</sub>	-10598	-9143	-6939	-4138	-703	5175
E <sub>3</sub>	-10598	-9143	-6939	-4138	-703	5075
g	.10358	.07077	.05436	.04538	.03928	.03241
h	.07067	.05344	.04323	.03715	.03290	.02846
s <sub>x</sub>	.00445	.00406	.00330	.00276	.00234	.00178
s <sub>y</sub>	.00003	.00010	.00022	.00029	.00032	.00011

**Table SIII f -**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.50$   $R(\text{OH}^3)=3.75$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5	6
$\varphi$	2.5	5	7.5	10	12.5	15
R(OH <sup>1</sup> )	1.8119	1.8179	1.8268	1.8374	1.8505	1.8717
R(OH <sup>2</sup> )	2.5000	2.5000	2.5000	2.5000	2.5000	2.5000
R(OH <sup>3</sup> )	3.7500	3.7500	3.7500	3.7500	3.7500	3.7500
R(H <sup>2</sup> H <sup>3</sup> )	1.9719	2.0445	2.1531	2.2934	2.4786	2.7890
R <sub>x</sub>	3.0305	3.0185	2.9995	2.9734	2.9361	2.8656
$\theta_1$	177	176	175	173	169	162
$\theta_2$	49	51	53	55	58	61
E <sub>1</sub>	-12890	-12949	-12949	-12831	-12521	-11684
E <sub>2</sub>	-11338	-9780	-7433	-4443	-693	4736
E <sub>3</sub>	-11338	-9780	-7433	-4443	-693	4736
g	.09931	.06519	.04994	.04202	.03652	.03069
h	.06752	.04976	.04026	.03484	.03106	.02713
s <sub>x</sub>	.00471	.00402	.00319	.00266	.00223	.00175
s <sub>y</sub>	.00007	.00008	.00019	.00026	.00028	.00004

**Table SIII g -**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.45$   $R(\text{OH}^3)=3.80$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5
$\varphi$	2.5	5	7.5	10	12.5
$R(\text{OH}^1)$	1.8118	1.8185	1.8282	1.8398	1.8558
$R(\text{OH}^2)$	2.4500	2.4500	2.4500	2.4500	2.4500
$R(\text{OH}^3)$	3.8000	3.8000	3.8000	3.8000	3.8000
$R(\text{H}^2\text{H}^3)$	1.9396	2.0194	2.1366	2.2876	2.4937
$R_x$	3.0464	3.0334	3.0133	2.9855	2.9439
$\theta_1$	178	176	175	172	168
$\theta_2$	44	46	49	52	55
$E_1$	-13535	-13667	-13737	-13670	-13358
$E_2$	-12042	-10346	-7825	-4609	-447
$E_3$	-12042	-10346	-7825	-4609	-447
$\ g\ $	.09230	.05832	.04497	.03828	.03346
$\ h\ $	.06315	.04534	.03690	.03232	.02905
$s_x$	.00496	.00385	.00300	.00249	.00209
$s_y$	.00011	.00004	.00015	.00022	.00022

**Table III h -**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.40$   $R(\text{OH}^3)=3.85$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5
$\varphi$	2.5	5	7.5	10	12.5
$R(\text{OH}^1)$	1.8130	1.8212	1.8308	1.8436	1.8638
$R(\text{OH}^2)$	2.4000	2.4000	2.4000	2.4000	2.4000
$R(\text{OH}^3)$	3.8500	3.8500	3.8500	3.8500	3.8500
$R(\text{H}^2\text{H}^3)$	1.9099	1.9999	2.1272	2.2913	2.5289
$R_x$	3.0626	3.0482	3.0267	2.9965	2.9483
$\theta_1$	178	176	174	171	166
$\theta_2$	39	42	45	49	53
$E_1$	-14150	-14382	-14537	-14526	-14191
$E_2$	-12676	-10795	-8060	-4573	180
$E_3$	-12676	-10794	-8060	-4573	180
$\ g\ $	.08122	.05022	.03960	.03439	.03025
$\ h\ $	.05689	.04011	.03323	.02964	.02688
$s_x$	.00505	.00352	.00272	.00228	.00189
$s_y$	.00015	.00000	.00011	.00017	.00014

**Table SIII i -**

Extension of 1,2 A' constrained  $R(\text{OH}^2)=2.35$   $R(\text{OH}^3)=3.90$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1	2	3	4	5
$\varphi$	2.5	5	7.5	10	12.5
$R(\text{OH}^1)$	1.8149	1.8249	1.8351	1.8496	1.8830
$R(\text{OH}^2)$	2.3500	2.3500	2.3500	2.3500	2.3500
$R(\text{OH}^3)$	3.9000	3.9000	3.9000	3.9000	3.9000
$R(\text{H}^2\text{H}^3)$	1.8847	1.9884	2.1280	2.3085	2.6052
$R_x$	3.0787	3.0623	3.0388	3.0057	2.9444
$\theta_1$	178	176	174	171	164
$\theta_2$	33	37	42	46	51
$E_1$	-14737	-15097	-15352	-15398	-14909
$E_2$	-13192	-11046	-8068	-4254	1552
$E_3$	-13192	-11046	-8068	-4254	1552
$\ g\ $	.06516	.04129	.00341	.03051	.02686
$\ h\ $	.04804	.03420	.02936	.02691	.02448
$s_x$	.00465	.00298	.00237	.00203	.00165
$s_y$	.00016	.00002	.00007	.00012	.00000

**Table III j -**

Extension of 1,2 A' constrained R(OH<sup>2</sup>)=2.30 R(OH<sup>3</sup>)=3.95 planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points

	1	2	3	4
$\varphi$	2.5	5	7.5	10
R(OH <sup>1</sup> )	1.8204	1.8311	1.8433	1.8594
R(OH <sup>2</sup> )	2.3000	2.3000	2.3000	2.3000
R(OH <sup>3</sup> )	3.9500	3.9500	3.9500	3.9500
R(H <sup>2</sup> H <sup>3</sup> )	1.8699	1.9903	2.1431	2.3442
R <sub>x</sub>	3.0939	3.0751	3.0493	3.0120
$\theta_1$	178	176	174	170
$\theta_2$	27	33	38	43
E <sub>1</sub>	-15323	-15840	-16175	-16274
E <sub>2</sub>	-13479	-11005	-7764	-3552
E <sub>3</sub>	-13479	-11005	-7764	-3552
g	.04485	.03234	.02884	.02683
h	.03611	.02797	.02553	.02424
s <sub>x</sub>	.00343	.00231	.00199	.00176
s <sub>y</sub>	.00014	.00004	.00003	.00006



**Table SIII k -**

Extension of 1,2 A' constrained  $R(OH^2)=2.25$   $R(OH^3)=4.00$  planar intersection to non-planar geometries resulting in seam of 2,3 A intersection points.

	1
$\varphi$	2.5
R(OH <sup>1</sup> )	1.8330
R(OH <sup>2</sup> )	2.2500
R(OH <sup>3</sup> )	4.0000
R(H <sup>2</sup> H <sup>3</sup> )	1.8786
R <sub>x</sub>	3.1063
$\theta_1$	178
$\theta_2$	20
E <sub>1</sub>	-15990
E <sub>2</sub>	-13282
E <sub>3</sub>	-13282
g	.02585
h	.02309
s <sub>x</sub>	.00177
s <sub>y</sub>	.00008

**Table SIV a -**

Extension of  $[R(H^2, H^3)] = [1.41072]$  asymptotote-like structures to the intersection region to nonplanar geometries.

	1	2	3	4	5	6
$\varphi$	0	2.5	5	7.5	10	12.5
R(OH <sup>1</sup> )	1.8480	1.8497	1.8578	1.8742	1.8779	1.8992
R(OH <sup>2</sup> )	2.7703	2.7593	2.7276	2.6814	2.6454	2.5823
R(OH <sup>3</sup> )	2.7703	2.7953	2.7276	3.6794	2.6454	2.5823
R(H <sup>2</sup> H <sup>3</sup> )	1.41072	1.41072	1.41072	1.41072	1.41072	1.41072
R <sub>x</sub>	2.6790	2.6676	2.6349	2.5859	2.5496	2.4840
$\theta_1$	180	180	180	180	180	180
$\theta_2$	90	90	90	90	90	90
E <sub>1</sub>	-10714	-10827	-11133	-11554	-12366	-12678
E <sub>2</sub>	-9158	-8682	-7275	-5048	-3010	451
E <sub>3</sub>	-9158	-8680	-7275	-5047	-3010	451
g	.13734	.11541	.08747	.07201	.06724	.06271
h	.10865	.09426	.07402	.06153	.05806	.05357
s <sub>x</sub>	.00893	.00822	.00687	.00636	.00628	.00623
s <sub>y</sub>	.00000	.00000	.00000	.00000	.00000	.00000

**Table SIV b -**Extension of 1,2<sup>2</sup>A' MEX to nonplanar regions with R(H<sup>2</sup>,H<sup>3</sup>) = [1.61072] constrained C<sub>2v</sub>MEX structure

	1	2	3	4	5	6	7
$\varphi$	2.5	5	7.5	10	12.5	15	17.5
R(OH <sup>1</sup> )	1.8481	1.8531	1.8623	1.8761	1.8956	1.9237	1.9620
R(OH <sup>2</sup> )	2.8375	2.8094	2.7665	2.7135	2.6550	2.5940	2.5844
R(OH <sup>3</sup> )	2.8375	2.8094	2.7665	2.7135	2.6550	2.5941	2.5845
R(H <sup>2</sup> H <sup>3</sup> )	1.59072	1.59072	1.59072	1.59072	1.59072	1.59072	1.59072
R <sub>x</sub>	2.7238	2.6945	2.6497	2.5943	2.5329	2.4692	2.4064
$\theta_1$	180	180	180	180	180	180	180
$\theta_2$	90	90	90	90	90	90	90
E <sub>1</sub>	-12029	-12381	-12896	-13484	-14052	-14500	-14741
E <sub>2</sub>	-9820	-8695	-6883	-4468	-1552	1752	5324
E <sub>3</sub>	-9820	-8695	-6883	-4468	-1552	1752	5324
g	.11402	.08957	.07423	.06614	.06235	.06122	.06183
h	.09256	.07492	.06275	.05566	.05173	.04966	.04868
s <sub>x</sub>	.00858	.00717	.00636	.00623	.00661	.00738	.00845
s <sub>y</sub>	.00000	.00000	.00000	.00000	.00000	.00000	.00000

**Table SVa -**

Extension of 2,3<sup>2</sup>A' symmetry-required MEX (D<sub>3H</sub>) to nonplanar regions as a function of  $\varphi$  between the D<sub>3h</sub> and C<sub>3v</sub> MEX structures.

	1	2	3	4	5	6	7	8	9	10
$\varphi$	5	10	15	20	25	30	36	41	46	51
R(OH <sup>1</sup> )	1.8423	1.8451	1.8479	1.8506	1.8534	1.8561	1.8588	1.8615	1.8643	1.8670
R(OH <sup>2</sup> )	1.8423	1.8451	1.8479	1.8506	1.8534	1.8561	1.8588	1.8615	1.8643	1.8670
R(OH <sup>3</sup> )	1.8423	1.8451	1.8479	1.8506	1.8534	1.8561	1.8588	1.8615	1.8643	1.8670
R(H <sup>2</sup> H <sup>3</sup> )	3.1896	3.1902	3.1879	3.1826	3.1742	3.1624	3.1472	3.1281	3.1049	3.0774
R <sub>x</sub>	0.9223	0.9279	0.9347	0.9446	0.9569	0.9718	0.9893	1.0094	1.0320	1.0573
$\theta_1$	180	180	180	180	180	180	180	180	180	180
$\theta_2$	90	90	90	90	90	90	90	90	90	90
E <sub>1</sub>	-28370	-28465	-28595	-28756	-28945	-29154	-29379	-29608	-29831	-30033
E <sub>2</sub>	-11654	-11699	-11734	-11874	-11993	-12126	-12260	-12385	-12484	-12537
E <sub>3</sub>	-11654	-11699	-11734	-11874	-11993	-12126	-12260	-12385	-12484	-12537
E <sub>4</sub>	-6923	-6943	-6987	-7050	-7125	-7205	-7278	-7331	-7348	-7307
g	.02481	.02516	.02559	.02610	.02668	.02734	.02809	.02891	.02982	.03079
h	.02481	.02516	.02559	.02610	.02668	.02734	.02809	.02891	.02982	.03079
s <sub>x</sub>	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
s <sub>y</sub>	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000

## Section SII-Cartesian Geometries for the MEXs

The Cartesian geometries for the structures reported in Table II and Tables from SI are presented below. The columns correspond to the atomic symbol, the atomic number, and the x y and z Cartesian components, respectively. Note left to right in the table corresponds to top to bottom in the Cartesian geometries lists below.

### C<sub>2v</sub> MEX

O	8.0	-0.05704157	-0.00000004	0.00000000
H	1.0	1.79021388	0.00000007	0.00000000
H	1.0	-2.80727537	0.79534403	0.00000000
H	1.0	-2.80727515	-0.79534385	0.00000000

### C<sub>∞v</sub> MEX

O	8.0	0.02953088	0.00000000	0.00000000
H	1.0	-1.78839364	0.00000000	0.00000000
H	1.0	2.27325285	0.00000000	0.00000000
H	1.0	4.05731850	0.00000000	0.00000000

### D<sub>3h</sub> MEX

O	8.0	-0.00877874	0.00000000	-0.00000078
H	1.0	1.83080046	-0.00000001	-0.00000083
H	1.0	-0.92856862	-0.00000001	1.59312338
H	1.0	-0.92856961	-0.00000001	-1.59312446

### C<sub>3v</sub> MEX

O	8.0	0.00881761	-0.00027295	0.00000000
H	1.0	0.60480175	-1.76833895	0.00000000
H	1.0	0.60549737	0.88352558	-1.53105462
H	1.0	0.60549738	0.88352558	1.53105463

**near~ C<sub>2v</sub> 1,2<sup>2</sup>A' planar MEXs**

**Table SIa**

O	8.0	-0.07093102	0.00068183	0.00000000
H	1.0	1.77978619	0.00999106	0.00000000
H	1.0	-2.76344388	0.76904015	0.00000000
H	1.0	-2.86133021	-0.78904749	0.00000000
O	8.0	0.21198740	0.00097246	0.00000000
H	1.0	-1.63917607	0.01401320	0.00000000
H	1.0	2.80560755	0.75139535	0.00000000
H	1.0	3.11121005	-0.77007102	0.00000000
O	8.0	0.19546234	0.00182273	0.00000000
H	1.0	-1.65650672	0.03182543	0.00000000
H	1.0	2.70088264	0.69671056	0.00000000
H	1.0	3.20210536	-0.75322545	0.00000000
O	8.0	0.19130880	0.00401097	0.00000000
H	1.0	-1.66203128	0.04791789	0.00000000
H	1.0	2.61229697	0.62756239	0.00000001
H	1.0	3.31035847	-0.71120167	0.00000001
O	8.0	0.18576465	0.00532267	0.00000000
H	1.0	-1.66976680	0.05646250	0.00000000
H	1.0	2.52497028	0.54208874	0.00000000
H	1.0	3.42284392	-0.63601688	0.00000001
O	8.0	0.16384374	0.01803601	0.00000006
H	1.0	-1.69185516	0.07886942	-0.00000013
H	1.0	2.42650390	0.43079499	-0.00000043
H	1.0	3.51626021	-0.54879831	-0.00000016

**near~C<sub>2v</sub> 1<sup>2</sup>A''/1<sup>2</sup>A' planar MEXs**

**Table SIb**

O	8.0	-0.07444875	0.06017231	0.00000000
H	1.0	1.80205066	-0.10842454	0.00000002
H	1.0	-2.87854138	0.56964707	0.00000066
H	1.0	-2.79526482	-0.78815542	-0.00000289
O	8.0	-0.07422903	0.06599658	0.00000001
H	1.0	1.80148689	-0.10874791	0.00000000
H	1.0	-2.82362415	0.59592719	-0.00000040
H	1.0	-2.85289930	-0.76405857	0.00000174
O	8.0	-0.07320278	0.06045108	-0.00000038
H	1.0	1.80404840	-0.08831065	0.00000066
H	1.0	-2.72465222	0.57017243	0.00000184
H	1.0	-2.95559175	-0.77131438	-0.00001511
O	8.0	-0.07127668	0.05448168	-0.00000002
H	1.0	1.80706444	-0.06423657	0.00000003

H	1.0	-2.62721064	0.53113834	0.00000039
H	1.0	-3.06200674	-0.76132081	-0.00000165
O	8.0	-0.06806462	0.04867046	-0.00000002
H	1.0	1.81064967	-0.03771358	0.00000001
H	1.0	-2.53061381	0.47977545	0.00000022
H	1.0	-3.17239240	-0.72795625	-0.00000083
O	8.0	-0.06351270	0.04372440	-0.00000001
H	1.0	1.81473398	-0.00864958	0.00000002
H	1.0	-2.43480526	0.41382113	-0.00000014
H	1.0	-3.28689108	-0.66326348	0.00000021
O	8.0	-0.05756931	0.04078042	0.00000001
H	1.0	1.81927563	0.02326758	0.00000004
H	1.0	-2.33974657	0.32655478	-0.00000036
H	1.0	-3.40559219	-0.55145502	0.00000060

**near~C<sub>∞v</sub> 1,2<sup>2</sup>A' planar MEXs**

**Table S1c**

O	8.0	0.03189632	0.01313066	0.00000000
H	1.0	-1.77775950	-0.00776376	0.00000000
H	1.0	2.27689072	0.16313114	0.00000000
H	1.0	4.02985641	-0.11460016	0.00000000
O	8.0	0.08913647	0.00309128	0.00000000
H	1.0	-1.72027265	-0.00392461	0.00000000
H	1.0	2.36699126	0.32148976	0.00000000
H	1.0	4.01689399	-0.41550266	0.00000000
O	8.0	0.09508462	-0.01115510	0.00000000
H	1.0	-1.71412433	-0.01908515	0.00000000
H	1.0	2.40572543	0.41714274	0.00000000
H	1.0	3.95356800	-0.57869892	0.00000000
O	8.0	0.05043947	-0.01341497	0.00000000
H	1.0	-1.75870307	-0.02819060	0.00000000
H	1.0	2.39302144	0.50841806	0.00000000
H	1.0	3.84202267	-0.68154432	0.00000000
O	8.0	0.05585016	-0.01745149	0.00000000
H	1.0	-1.75343979	-0.03505228	0.00000000
H	1.0	2.43196614	0.57968572	0.00000000
H	1.0	3.77981206	-0.77382956	0.00000000
O	8.0	0.06142873	0.00460831	0.00000000
H	1.0	-1.74832129	0.00415410	0.00000000
H	1.0	2.47884782	0.64185624	0.00000000
H	1.0	3.70908402	-0.86551288	0.00000000
O	8.0	0.06605650	-0.02485481	0.00000000
H	1.0	-1.74413236	-0.04761220	0.00000000
H	1.0	2.51115338	0.69902447	0.00000000

H	1.0	3.65678974	-0.91739879	0.00000000
O	8.0	0.07126282	0.00456847	0.00000000
H	1.0	-1.73985098	0.00258343	0.00000000
H	1.0	2.56148067	0.75210783	0.00000000
H	1.0	3.58436814	-0.98567945	0.00000000
O	8.0	0.07532000	-0.03195406	0.00000000
H	1.0	-1.73653976	-0.06059376	0.00000000
H	1.0	2.59111303	0.80068356	0.00000000
H	1.0	3.53737075	-1.01897208	0.00000000
O	8.0	0.07976974	-0.00052386	0.00000000
H	1.0	-1.73341552	-0.01296230	0.00000000
H	1.0	2.64073603	0.85472553	0.00000000
H	1.0	3.46857462	-1.05811626	0.00000000
O	8.0	0.08375385	-0.04052517	0.00000000
H	1.0	-1.73045870	-0.07345197	0.00000000
H	1.0	2.67277652	0.88654636	0.00000000
H	1.0	3.42199145	-1.09227120	0.00000000

**near~C<sub>∞v</sub> 1<sup>2</sup>A<sup>1</sup> / 1<sup>2</sup>A<sup>1</sup> planar MEXs**

**Table SId**

O	8.0	0.03943867	0.01679136	0.00000000
H	1.0	-1.82196920	-0.00879126	0.00000000
H	1.0	2.28922481	0.04781299	0.00000000
H	1.0	4.03906144	0.07172486	0.00000000
O	8.0	0.03931406	0.01909778	0.00000000
H	1.0	-1.81970670	-0.03118856	0.00000000
H	1.0	2.33847052	0.08138402	0.00000000
H	1.0	3.98786718	0.12600096	0.00000000
O	8.0	0.03967004	0.02273510	0.00000000
H	1.0	-1.81646927	-0.06010685	0.00000000
H	1.0	2.38670423	0.14076266	0.00000000
H	1.0	3.93565934	0.19956095	0.00000000
O	8.0	0.04009066	0.01928679	0.00000000
H	1.0	-1.81446389	-0.06373788	0.00000000
H	1.0	2.43554930	0.16686013	0.00000000
H	1.0	3.88552824	0.20666297	0.00000000
O	8.0	0.04067951	-0.03635330	0.00000000
H	1.0	-1.81375981	0.04533605	0.00000000
H	1.0	2.47537493	0.23706625	0.00000000
H	1.0	3.84066094	-0.04823256	0.00000000
O	8.0	0.04304714	-0.07565820	0.00000000
H	1.0	-1.80537373	0.10156096	0.00000000
H	1.0	2.51038674	0.32712622	0.00000000
H	1.0	3.79102451	-0.19880672	0.00000000



O	8.0	0.04478111	-0.10045467	0.00000000
H	1.0	-1.79681311	0.14197370	0.00000000
H	1.0	2.54940282	0.37847128	0.00000000
H	1.0	3.73807608	-0.32310289	0.00000000
O	8.0	0.04573447	-0.13890258	0.00000000
H	1.0	-1.77990956	0.20812590	0.00000000
H	1.0	2.58048460	0.43992536	0.00000000
H	1.0	3.68828610	-0.37196399	0.00000000
O	8.0	0.04737534	-0.15062815	0.00000000
H	1.0	-1.77353268	0.22203928	0.00000000
H	1.0	2.62278689	0.47367574	0.00000000
H	1.0	3.63475167	-0.45184405	0.00000000
O	8.0	0.05303953	-0.16301685	0.00000000
H	1.0	-1.76577714	0.22217169	0.00000000
H	1.0	2.70746319	0.55568686	0.00000000
H	1.0	3.53321064	-0.53505049	0.00000000

**near- $C_{2v}$  out-of-plane MEXs**  
**Table SIIa**

O	8.	-0.05812396	0.00000001	-0.00605791
H	1.	1.78826012	0.00000000	0.05750142
H	1.	-2.80551062	0.80473058	0.01928170
H	1.	-2.80551048	-0.80473054	0.01928171
O	8.	-0.06130635	0.00000000	-0.01212549
H	1.	1.78280303	0.00000000	0.11498854
H	1.	-2.80051745	0.83098499	0.03840523
H	1.	-2.80051731	-0.83098496	0.03840523
O	8.	-0.06656075	0.00000000	-0.01823125
H	1.	1.77515538	-0.00000001	0.17249345
H	1.	-2.79298059	0.87022482	0.05733635
H	1.	-2.79298046	-0.87022479	0.05733637
O	8.	-0.07751062	-0.00000001	-0.02444855
H	1.	1.76429529	0.00000001	0.23027893
H	1.	-2.77678030	0.94882635	0.07574489
H	1.	-2.77678016	-0.94882629	0.07574510
O	8.	-0.08681521	-0.00000001	-0.03076528
H	1.	1.75411965	0.00000003	0.28803764
H	1.	-2.76505419	1.00386357	0.09437830
H	1.	-2.76505408	-1.00386345	0.09437862
O	8.	-0.09715072	-0.00000001	-0.03715020
H	1.	1.74130456	0.00000002	0.34568415
H	1.	-2.75181886	1.06139701	0.11298744
H	1.	-2.75181878	-1.06139679	0.11298781

O	8.	-0.10890641	0.00000117	-0.04368440
H	1.	1.72714609	-0.00000112	0.40340313
H	1.	-2.73695284	1.12207779	0.13148085
H	1.	-2.73698559	-1.12197919	0.13160420
O	8.	-0.12394210	0.00000000	-0.05069718
H	1.	1.71532751	0.00000004	0.46217042
H	1.	-2.71948303	1.19134233	0.14989596
H	1.	-2.71948291	-1.19134228	0.14989590

**R(OH<sup>2</sup>)=2.80 R(OH<sup>3</sup>)=2.90 out-of-plane MEXs**  
**Table SIIB**

O	8.	-0.07197837	0.00075992	-0.00606770
H	1.	1.77765688	0.00984223	0.05748441
H	1.	-2.76175993	0.77821789	0.01911590
H	1.	-2.85941256	-0.79895915	0.01962251
O	8.	-0.07508522	0.00095275	-0.01213901
H	1.	1.77184568	0.00945516	0.11493967
H	1.	-2.75705018	0.80383218	0.03734433
H	1.	-2.85399848	-0.82666060	0.03979696
O	8.	-0.08019236	0.00120249	-0.01823434
H	1.	1.76357117	0.00888476	0.17237706
H	1.	-2.75000774	0.84189448	0.05472320
H	1.	-2.84575288	-0.86798536	0.06042640
O	8.	-0.09091250	0.00185900	-0.02443982
H	1.	1.75244507	0.00703141	0.23009901
H	1.	-2.73540281	0.91721278	0.06936067
H	1.	-2.82833655	-0.94945910	0.08281485
O	8.	-0.10019379	0.00170195	-0.03173514
H	1.	1.74252211	0.00705880	0.28900865
H	1.	-2.72420201	0.97345350	0.06965509
H	1.	-2.81664028	-1.00335956	0.11238338
O	8.	-0.11045902	0.00281565	-0.03831535
H	1.	1.73008585	0.00414244	0.34700767
H	1.	-2.71198804	1.03068266	0.08633314
H	1.	-2.80283835	-1.06123678	0.13164687
O	8.	-0.12168060	0.00435057	-0.04437167
H	1.	1.71441221	-0.00083602	0.40403750
H	1.	-2.69918198	1.08702906	0.11149335
H	1.	-2.78558741	-1.12573933	0.14667126
O	8.	-0.13652092	0.00585160	-0.05036626
H	1.	1.70298882	-0.00454631	0.46116086
H	1.	-2.67846357	1.16966467	0.10476857
H	1.	-2.77249316	-1.17658322	0.20162254

**R(OH<sup>2</sup>)=2.70 R(OH<sup>3</sup>)=3.00 out-of-plane MEXs**

**Table SIIC**

O	8.	0.21402076	0.00197806	0.00606366
H	1.	-1.63324645	0.01192997	-0.05745773
H	1.	2.80079267	0.77528264	-0.01865642
H	1.	3.10410644	-0.80221645	-0.01993489
O	8.	0.21770089	0.00288016	0.01329875
H	1.	-1.62717659	0.01329596	-0.11492111
H	1.	2.79672410	0.80101727	-0.02690602
H	1.	3.09638375	-0.83966341	-0.04419366
O	8.	0.22365041	0.00360040	0.01839353
H	1.	-1.61980474	0.00796478	-0.17265791
H	1.	2.78903815	0.84283274	-0.04850087
H	1.	3.08701985	-0.88756160	-0.06494740
O	8.	0.23157735	0.00419651	0.02508178
H	1.	-1.61188018	0.00591572	-0.23118011
H	1.	2.78112369	0.88959908	-0.05157195
H	1.	3.07461459	-0.94580118	-0.09592937
O	8.	0.24074608	0.00543045	0.03199594
H	1.	-1.60129700	0.00194666	-0.28981761
H	1.	2.77209341	0.94053452	-0.05666804
H	1.	3.06022649	-1.00753099	-0.12433529
O	8.	0.25087622	0.00770170	0.03884348
H	1.	-1.58763369	-0.00523141	-0.34811759
H	1.	2.76185354	0.99469456	-0.06526768
H	1.	3.04379245	-1.07101710	-0.15085649
O	8.	0.26240426	0.01110956	0.04459225
H	1.	-1.57207014	-0.01747636	-0.40476997
H	1.	2.75215337	1.04718847	-0.08841102
H	1.	3.02269114	-1.14378584	-0.17227844
O	8.	0.27766190	0.01521363	0.05084119
H	1.	-1.56053229	-0.03441789	-0.46268893
H	1.	2.74302641	1.10499675	-0.10520558
H	1.	2.99593723	-1.22842415	-0.20282057

**R(OH<sup>2</sup>)=2.60 R(OH<sup>3</sup>)=3.10 out-of-plane MEXs****Table SIId**

O	8.	0.19648708	0.00221257	0.00607604
H	1.	-1.65414220	0.03109473	-0.05769750
H	1.	2.69952765	0.70521641	-0.01787141
H	1.	3.19972576	-0.76580108	-0.02061553
O	8.	0.19955282	0.00313042	0.01217142
H	1.	-1.64780058	0.02925891	-0.11543762
H	1.	2.69587405	0.72870816	-0.03161418
H	1.	3.19294001	-0.80086871	-0.04456071

O	8.	0.20462479	0.00430989	0.01829366
H	1.	-1.63859631	0.02646847	-0.17321748
H	1.	2.69066297	0.76323010	-0.04215664
H	1.	3.18214754	-0.85379327	-0.07124561
O	8.	0.21488082	0.00696433	0.02454216
H	1.	-1.62678481	0.01830752	-0.23147453
H	1.	2.68111715	0.82728445	-0.04440267
H	1.	3.16047726	-0.95026107	-0.10653560
O	8.	0.22415573	0.00882173	0.03105432
H	1.	-1.61570074	0.01109932	-0.28993920
H	1.	2.67489773	0.87312818	-0.05164085
H	1.	3.14239853	-1.02355606	-0.13644444
O	8.	0.23463417	0.01164973	0.03711484
H	1.	-1.60206387	-0.00061738	-0.34757740
H	1.	2.66867059	0.92000623	-0.06464524
H	1.	3.12049227	-1.10217091	-0.16592844
O	8.	0.24679380	0.01549228	0.04348143
H	1.	-1.58692930	-0.01921094	-0.40570619
H	1.	2.66195899	0.97091026	-0.07548700
H	1.	3.09480887	-1.18468168	-0.19816416
O	8.	0.26306492	0.02177698	0.05030639
H	1.	-1.57437694	-0.05062939	-0.46527853
H	1.	2.65512840	1.03177497	-0.08361994
H	1.	3.06153408	-1.28001216	-0.23937506

**R(OH<sup>2</sup>)=2.50 R(OH<sup>3</sup>)=3.20 out-of-plane MEXs**  
**Table SIIe**

O	8.	0.19232893	0.00454020	0.00608626
H	1.	-1.65940263	0.04689610	-0.05791636
H	1.	2.61106817	0.63633823	-0.01697424
H	1.	3.30763727	-0.72628659	-0.02122698
O	8.	0.19539757	0.00569709	0.01220656
H	1.	-1.65245419	0.04443179	-0.11595105
H	1.	2.60786858	0.66019593	-0.02797926
H	1.	3.29987364	-0.76806155	-0.04717188
O	8.	0.20054640	0.00720615	0.01832930
H	1.	-1.64201592	0.04033105	-0.17404158
H	1.	2.60340100	0.69527563	-0.03505907
H	1.	3.28696803	-0.83240318	-0.07684249
O	8.	0.21056225	0.01017205	0.02454354
H	1.	-1.62964807	0.02958295	-0.23262361
H	1.	2.59636568	0.75466459	-0.03606283
H	1.	3.26302432	-0.94019356	-0.11431205

O	8.	0.22024040	0.01242661	0.03065080
H	1.	-1.61861624	0.01865147	-0.29092682
H	1.	2.59254512	0.79749268	-0.04577999
H	1.	3.24122672	-1.02795481	-0.14612054
O	8.	0.23124798	0.01540853	0.03657466
H	1.	-1.60448921	0.00080885	-0.34893962
H	1.	2.58885622	0.84164044	-0.05842131
H	1.	3.21458091	-1.12196725	-0.17813657
O	8.	0.24441040	0.01936442	0.04230667
H	1.	-1.58881664	-0.02807383	-0.40699017
H	1.	2.58528440	0.88947992	-0.07261969
H	1.	3.18181391	-1.22404712	-0.21379558
O	8.	0.26290847	0.03015283	0.05077430
H	1.	-1.57700819	-0.07900950	-0.47234401
H	1.	2.57268107	0.98146455	-0.04900895
H	1.	3.14934713	-1.30681142	-0.29707407

**R(OH<sup>2</sup>)=2.40 R(OH<sup>3</sup>)=3.30 out-of-plane MEXs  
Table SIIf**

O	8.	0.18680432	0.00594011	0.00610371
H	1.	-1.66671982	0.05518253	-0.05822405
H	1.	2.52374687	0.55204064	-0.01568025
H	1.	3.41969075	-0.65561235	-0.02204660
O	8.	0.18989701	0.00715572	0.01224766
H	1.	-1.65830089	0.05211924	-0.11665124
H	1.	2.52062249	0.57851307	-0.02339401
H	1.	3.41043317	-0.70994706	-0.05027564
O	8.	0.19732621	0.00940713	0.01838940
H	1.	-1.64559374	0.04297633	-0.17548106
H	1.	2.51489952	0.63169237	-0.02180851
H	1.	3.38966833	-0.81970991	-0.08892017
O	8.	0.20565682	0.01103408	0.02429707
H	1.	-1.63512186	0.03346250	-0.23381898
H	1.	2.51231150	0.67136013	-0.03327458
H	1.	3.36843363	-0.91978613	-0.11858462
O	8.	0.21599719	0.01293460	0.02981874
H	1.	-1.62364875	0.01711632	-0.29174923
H	1.	2.51104758	0.71032428	-0.05013196
H	1.	3.34147355	-1.03115124	-0.14704510
O	8.	0.22824749	0.01469968	0.03464141
H	1.	-1.60946500	-0.01021738	-0.34899956
H	1.	2.51088133	0.74822681	-0.07269664
H	1.	3.30716654	-1.15428025	-0.17450439
O	8.	0.23422898	0.02256771	0.02629375

H	1.	-1.60334403	-0.05721746	-0.38304907
H	1.	2.52411445	0.76475902	-0.16135248
H	1.	3.28846102	-1.34400793	-0.16056379
O	8.	0.29631528	-0.02335626	-0.00424966
H	1.	-1.64153880	-0.16734402	-0.37000722
H	1.	2.49774194	0.90908861	-0.21464925
H	1.	3.19465843	-1.34578183	-0.86494484

**R(OH<sup>2</sup>)=2.30 R(OH<sup>3</sup>)=3.40 out-of-plane MEXs**  
**Table SIIg**

O	8.	0.16535542	0.01836607	0.00610999
H	1.	-1.68788079	0.07684366	-0.05844088
H	1.	2.42468866	0.44846124	-0.01468551
H	1.	3.51137556	-0.58439424	-0.02264095
O	8.	0.16958899	0.01871580	0.01220220
H	1.	-1.67854693	0.07220248	-0.11712455
H	1.	2.42113557	0.48713521	-0.02129747
H	1.	3.49823481	-0.67117821	-0.05230075
O	8.	0.17658888	0.01908361	0.01796449
H	1.	-1.66897317	0.06384611	-0.17541624
H	1.	2.41877845	0.52898809	-0.03287171
H	1.	3.47857524	-0.78534534	-0.08091653
O	8.	0.18626929	0.01924548	0.02298220
H	1.	-1.65953194	0.04822680	-0.23198959
H	1.	2.41961151	0.56227301	-0.06248466
H	1.	3.45046378	-0.92468252	-0.09547246
O	8.	0.19784261	0.01757572	0.02700866
H	1.	-1.64708952	0.02106306	-0.28853107
H	1.	2.42097710	0.59618080	-0.08652647
H	1.	3.41554913	-1.07077754	-0.12080669
O	8.	0.21795226	0.03466462	0.01119057
H	1.	-1.63518797	-0.02472956	-0.31517822
H	1.	2.42722566	0.62439501	-0.23645839
H	1.	3.36760350	-1.23752563	-0.13450199
O	8.	0.23656025	0.01219300	0.02149056
H	1.	-1.61683551	-0.11136312	-0.38410669
H	1.	2.43005793	0.66562257	-0.20566280
H	1.	3.31093736	-1.42687880	-0.17157685

**R(OH<sup>2</sup>)=2.25 R(OH<sup>3</sup>)=4.00 out-of-plane MEXs**  
**Table SIIIa**

O	8.	0.04115000	0.00530328	0.00566218
H	1.	-1.79055113	-0.02568113	-0.05645850
H	1.	2.27308165	0.28509776	-0.04626264
H	1.	4.02038040	-0.40140607	0.02334896

**R(OH<sup>2</sup>)=2.30 R(OH<sup>3</sup>)=3.95 out-of-plane MEXs  
Table SIIIb**

O	8.	0.09441169	0.00294571	0.00588662
H	1.	-1.72477458	-0.01257312	-0.05853332
H	1.	2.36509599	0.36832187	-0.01632019
H	1.	4.00923066	-0.52239627	-0.02072822
O	8.	0.10349536	0.00435981	0.01140219
H	1.	-1.72268549	-0.03407703	-0.11712252
H	1.	2.36144220	0.44050197	-0.02675705
H	1.	3.98867335	-0.70517645	-0.05530816
O	8.	0.11583624	0.00657470	0.01673425
H	1.	-1.71574709	-0.07267039	-0.17538265
H	1.	2.35856286	0.51350224	-0.03986193
H	1.	3.95526910	-0.91498135	-0.09276507
O	8.	0.13360697	0.00207341	0.02338019
H	1.	-1.70219895	-0.14085750	-0.23516831
H	1.	2.35909463	0.57793544	-0.05136986
H	1.	3.89653752	-1.19029756	-0.12189576

**R(OH<sup>2</sup>)=2.35 R(OH<sup>3</sup>)=3.90 out-of-plane MEXs  
Table SIIIc**

O	8.	0.09854258	-0.01002089	0.00588493
H	1.	-1.71516274	-0.02558550	-0.05839213
H	1.	2.40439321	0.44282026	-0.01620004
H	1.	3.94731323	-0.63950251	-0.02089660
O	8.	0.10653500	-0.00714088	0.01153736
H	1.	-1.71342389	-0.04239608	-0.11728203
H	1.	2.40143936	0.49772279	-0.02050433
H	1.	3.92974581	-0.77360834	-0.06320678
O	8.	0.11758160	-0.00229048	0.01691814
H	1.	-1.70600006	-0.07102870	-0.17635925
H	1.	2.39788721	0.56441137	-0.02252127
H	1.	3.90095876	-0.93869914	-0.12163159
O	8.	0.13310792	0.00493211	0.02251637
H	1.	-1.69405198	-0.11894450	-0.23630402
H	1.	2.39418433	0.64362978	-0.02331919
H	1.	3.85649054	-1.13394215	-0.19971713
O	8.	0.16227625	0.01759746	0.02997643
H	1.	-1.67657424	-0.21362269	-0.30268333
H	1.	2.39070290	0.76293425	-0.00300602
H	1.	3.76515556	-1.41750167	-0.38203220

**R(OH<sup>2</sup>)=2.40 R(OH<sup>3</sup>)=3.85 out-of-plane MEXs  
Table SIIId**

O	8.	0.05310465	-0.01196670	0.00589057
H	1.	-1.75861044	-0.03356534	-0.05828708
H	1.	2.39197623	0.52576739	-0.01695128
H	1.	3.83671621	-0.72338640	-0.01990598
O	8.	0.06002814	-0.00841399	0.01162573
H	1.	-1.75622101	-0.04794204	-0.11705241
H	1.	2.38936979	0.56870474	-0.02156267
H	1.	3.82135981	-0.82680809	-0.05989446
O	8.	0.07012559	-0.00300710	0.01714163
H	1.	-1.74915277	-0.07162074	-0.17623792
H	1.	2.38586616	0.62624966	-0.02002813
H	1.	3.79592380	-0.96330041	-0.11984185
O	8.	0.08411564	0.00517090	0.02270630
H	1.	-1.73762028	-0.10972651	-0.23622852
H	1.	2.38170352	0.69769168	-0.01609422
H	1.	3.75761368	-1.12510015	-0.20179210
O	8.	0.10597509	0.01910961	0.02914687
H	1.	-1.71804998	-0.17721912	-0.29964092
H	1.	2.37599927	0.79763386	-0.00068943
H	1.	3.69034433	-1.33513464	-0.34611248

**R(OH<sup>2</sup>)=2.45 R(OH<sup>3</sup>)=3.80 out-of-plane MEXs  
Table SIIIe**

O	8.	0.05802850	-0.01595841	0.00589334
H	1.	-1.75252551	-0.03968099	-0.05820813
H	1.	2.43105255	0.59289780	-0.01757892
H	1.	3.77500061	-0.80557432	-0.01910848
O	8.	0.06414915	-0.01217953	0.01167190
H	1.	-1.74934753	-0.05239508	-0.11680092
H	1.	2.42869086	0.62828445	-0.02366080
H	1.	3.76099481	-0.88897785	-0.05583252
O	8.	0.07365276	-0.00656159	0.01731005
H	1.	-1.74310837	-0.07309064	-0.17591752
H	1.	2.42548803	0.67889437	-0.02168893
H	1.	3.73793276	-1.00464827	-0.11259325
O	8.	0.08651108	0.00160907	0.02293698
H	1.	-1.73186248	-0.10521737	-0.23573349
H	1.	2.42131974	0.74299998	-0.01590038
H	1.	3.70363514	-1.14326958	-0.19076017
O	8.	0.10517147	0.01480322	0.02908221
H	1.	-1.71332414	-0.15885022	-0.29783247
H	1.	2.41549307	0.82964419	-0.00174540
H	1.	3.64812051	-1.31543377	-0.31440282



**R(OH<sup>2</sup>)=2.50 R(OH<sup>3</sup>)=3.75 out-of-plane MEXs****Table SIIIIf**

O	8.	0.06344179	0.00605609	0.00590102
H	1.	-1.74733757	0.00001325	-0.05816769
H	1.	2.47817781	0.65295477	-0.01801640
H	1.	3.70442368	-0.89124653	-0.01857014
O	8.	0.06918317	0.00981883	0.01172001
H	1.	-1.74405904	-0.01153019	-0.11665446
H	1.	2.47634558	0.68374789	-0.02554616
H	1.	3.69084652	-0.96070669	-0.05258119
O	8.	0.07818294	0.01539019	0.01743681
H	1.	-1.73777022	-0.03020698	-0.17561817
H	1.	2.47366228	0.72949106	-0.02426016
H	1.	3.66865827	-1.05973340	-0.10542960
O	8.	0.09034361	0.02327546	0.02314155
H	1.	-1.72697048	-0.05851715	-0.23522294
H	1.	2.47002918	0.78839460	-0.01796204
H	1.	3.63641440	-1.17974259	-0.17842633
O	8.	0.10711008	0.03544029	0.02916732
H	1.	-1.70915802	-0.10380139	-0.29642770
H	1.	2.46476803	0.86629680	-0.00441053
H	1.	3.58711120	-1.32539310	-0.28741579
O	8.	0.13699129	0.06102551	0.03760256
H	1.	-1.67257684	-0.19559151	-0.36595150
H	1.	2.45627058	0.99426725	0.03576214
H	1.	3.48209856	-1.53811259	-0.52410448

**R(OH<sup>2</sup>)=2.55 R(OH<sup>3</sup>)=3.70 out-of-plane MEXs****Table SIIIg**

O	8.	0.06789661	-0.02346672	0.00590901
H	1.	-1.74307662	-0.05130577	-0.05814640
H	1.	2.51039347	0.70873585	-0.01834814
H	1.	3.65267499	-0.93931863	-0.01815690
O	8.	0.07320270	-0.01977863	0.01176219
H	1.	-1.73965274	-0.06169001	-0.11656190
H	1.	2.50825879	0.73618144	-0.02730564
H	1.	3.64059589	-0.99953908	-0.04968153
O	8.	0.08158801	-0.01427282	0.01754464
H	1.	-1.73318742	-0.07841681	-0.17539009
H	1.	2.50503641	0.77779571	-0.02745858
H	1.	3.62071667	-1.08720166	-0.09817891
O	8.	0.09277616	-0.00659821	0.02329439
H	1.	-1.72174974	-0.10325214	-0.23469474
H	1.	2.50061592	0.83170582	-0.02202677

H	1.	3.59179107	-1.19467082	-0.16479626
O	8.	0.10820757	0.00489280	0.02930847
H	1.	-1.70527439	-0.14182733	-0.29532673
H	1.	2.49485324	0.90205214	-0.00978197
H	1.	3.54897484	-1.32429396	-0.26117907
O	8.	0.16098154	0.08941021	0.05128490
H	1.	-1.66431678	-0.31637454	-0.30581965
H	1.	2.52557629	1.01177433	-0.19455264
H	1.	3.36871808	-1.74863612	0.19964924

**R(OH<sup>2</sup>)=2.60 R(OH<sup>3</sup>)=3.65 out-of-plane MEXs  
Table SIIIh**

O	8.	0.07307681	0.00584031	0.00590926
H	1.	-1.73877927	-0.00082633	-0.05814755
H	1.	2.56111159	0.76144013	-0.01827158
H	1.	3.57987944	-1.00493585	-0.01831751
O	8.	0.07823286	0.00932151	0.01178660
H	1.	-1.73541277	-0.01033133	-0.11652955
H	1.	2.55924948	0.78700485	-0.02818861
H	1.	3.56795657	-1.05751917	-0.04820898
O	8.	0.08638819	0.01456161	0.01762642
H	1.	-1.72909725	-0.02566104	-0.17528122
H	1.	2.55635071	0.82628458	-0.02953218
H	1.	3.54849597	-1.13496717	-0.09334000
O	8.	0.09726245	0.02180720	0.02345950
H	1.	-1.71829276	-0.04817665	-0.23446809
H	1.	2.55233196	0.87745459	-0.02485435
H	1.	3.52068802	-1.23049981	-0.15487904
O	8.	0.11190293	0.03238718	0.02950343
H	1.	-1.70283816	-0.08230280	-0.29471234
H	1.	2.54707061	0.94340205	-0.01343285
H	1.	3.48085733	-1.34476323	-0.24164821
O	8.	0.14540383	0.05659226	0.03857599
H	1.	-1.70060530	-0.15775086	-0.36580288
H	1.	2.54367190	1.06162806	0.03177790
H	1.	3.39723333	-1.52793316	-0.44598998

**R(OH<sup>2</sup>)=2.65 R(OH<sup>3</sup>)=3.60 out-of-plane MEXs  
Table SIIIi**

O	8.	0.07700457	-0.03073971	0.00592551
H	1.	-1.73546071	-0.06361164	-0.05814674
H	1.	2.59030866	0.80901885	-0.01873574
H	1.	3.53373104	-1.03596835	-0.01768619

O	8.	0.08190301	-0.02742351	0.01183428
H	1.	-1.73203995	-0.07220017	-0.11649706
H	1.	2.58799217	0.83296708	-0.02994146
H	1.	3.52303429	-1.08351500	-0.04549232
O	8.	0.08966887	-0.02238931	0.01772576
H	1.	-1.72566274	-0.08602138	-0.17516536
H	1.	2.58438249	0.86998618	-0.03296869
H	1.	3.50550475	-1.15425824	-0.08685887
O	8.	0.10002507	-0.01545569	0.02362196
H	1.	-1.71499938	-0.10608843	-0.23419631
H	1.	2.57951304	0.91823446	-0.02987714
H	1.	3.48047310	-1.24218780	-0.14280937
O	8.	0.11375906	-0.00549283	0.02968211
H	1.	-1.69980917	-0.13592998	-0.29403750
H	1.	2.57330997	0.97970362	-0.02029349
H	1.	3.44502093	-1.34726286	-0.22001284
O	8.	0.13816305	0.01386017	0.03706959
H	1.	-1.68270980	-0.19321637	-0.35888063
H	1.	2.56536054	1.07714679	0.01186532
H	1.	3.37912331	-1.49930107	-0.37099878

**R(OH<sup>2</sup>)=2.70 R(OH<sup>3</sup>)=3.55 out-of-plane MEXs  
Table SIIIj**

O	8.	0.08139074	0.00060790	0.00593672
H	1.	-1.73239816	-0.01560966	-0.05817796
H	1.	2.63954380	0.86229496	-0.01842664
H	1.	3.46558261	-1.07309884	-0.01804158
O	8.	0.08622521	0.00365714	0.01187586
H	1.	-1.72908268	-0.02340156	-0.11654335
H	1.	2.63726824	0.88550409	-0.03020449
H	1.	3.45510040	-1.11600609	-0.04478021
O	8.	0.09371335	0.00830947	0.01780421
H	1.	-1.72219606	-0.03593933	-0.17514202
H	1.	2.63355992	0.92137939	-0.03442598
H	1.	3.43793540	-1.18001989	-0.08332885
O	8.	0.10405038	0.01474608	0.02380346
H	1.	-1.71272246	-0.05414863	-0.23418003
H	1.	2.62886817	0.96835424	-0.03251628
H	1.	3.41396172	-1.26020225	-0.13484496
O	8.	0.11735488	0.02385243	0.02993495
H	1.	-1.69834056	-0.08078825	-0.29382680
H	1.	2.62275265	1.02749271	-0.02422834
H	1.	3.38059451	-1.35545826	-0.20446811
O	8.	0.13886624	0.04021348	0.03695746

H	1.	-1.68084602	-0.12843141	-0.35677260
H	1.	2.61465727	1.11561779	0.00216290
H	1.	3.32351122	-1.48659511	-0.32782707

**R(OH<sup>2</sup>)=2.75 R(OH<sup>3</sup>)=3.50 out-of-plane MEXs**  
**Table SIIIk**

O	8.	0.08536538	-0.03951352	0.00594379
H	1.	-1.72941137	-0.07587354	-0.05819338
H	1.	2.67182741	0.89434808	-0.01888818
H	1.	3.41874125	-1.10631042	-0.01750131
O	8.	0.09005829	-0.03669801	0.01190262
H	1.	-1.72612003	-0.08282556	-0.11655976
H	1.	2.66909066	0.91681030	-0.03184569
H	1.	3.40920038	-1.14590384	-0.04248603
O	8.	0.09734370	-0.03237238	0.01787148
H	1.	-1.71939409	-0.09400226	-0.17513787
H	1.	2.66469344	0.95155406	-0.03784212
H	1.	3.39356323	-1.20532020	-0.07768062
O	8.	0.10732334	-0.02639540	0.02391690
H	1.	-1.70999646	-0.11011264	-0.23408287
H	1.	2.65911084	0.99685927	-0.03797318
H	1.	3.37177219	-1.27998734	-0.12400511
O	8.	0.12006033	-0.01803345	0.03007807
H	1.	-1.69596691	-0.13334707	-0.29349554
H	1.	2.65201133	1.05335818	-0.03192398
H	1.	3.34173536	-1.36870207	-0.18557053
O	8.	0.13963256	-0.00377655	0.03689614
H	1.	-1.67905766	-0.17303396	-0.35526929
H	1.	2.64266713	1.13422787	-0.01069255
H	1.	3.29301777	-1.48730953	-0.28759085

**constrained R(H<sup>2</sup>H<sup>3</sup>)=1.41072 to out-of-plane MEXs**  
**Table SIVa**

O	8.0	-0.08062834	-0.00000001	0.00000000
H	1.0	1.76738382	0.00000043	0.00000000
H	1.0	-2.75965514	0.70535958	0.00000000
H	1.0	-2.75966058	-0.70536042	0.00000000
O	8.	-0.08782692	0.00000002	-0.00597706
H	1.	1.76078452	0.00000001	0.05729840
H	1.	-2.75536660	0.70536029	0.01914581
H	1.	-2.75536769	-0.70536037	0.01914582

O	8.	-0.11057280	0.00000003	-0.01195906
H	1.	1.74294469	0.00000032	0.11443291
H	1.	-2.74493487	0.70536013	0.03857723
H	1.	-2.74494298	-0.70536053	0.03857693
O	8.	-0.14809380	-0.00001970	-0.01800047
H	1.	1.71655064	-0.00007146	0.17140560
H	1.	-2.73391963	0.70541591	0.05869022
H	1.	-2.73187906	-0.70530328	0.05873430
O	8.	-0.18516062	0.00000142	-0.02371250
H	1.	1.67594167	0.00000364	0.22696286
H	1.	-2.73263958	0.70535726	0.07989427
H	1.	-2.73274425	-0.70536340	0.07989328
O	8.	-0.24596848	-0.00000052	-0.02956365
H	1.	1.62746148	-0.00000067	0.28247682
H	1.	-2.72651389	0.70536150	0.10232611
H	1.	-2.72648609	-0.70535916	0.10232685
O	8.	-0.32172645	-0.00000002	-0.03574716
H	1.	1.57607299	-0.00000004	0.33849462
H	1.	-2.73149637	0.70536023	0.12619007
H	1.	-2.73149644	-0.70536043	0.12618988

**constrained  $R(H^2H^3)=1.59102$  to out-of-plane MEXs**  
**Table SIVb**

O	8.	-0.06831507	0.00000000	-0.00603105
H	1.	1.77871345	0.00000001	0.05741706
H	1.	-2.79197180	0.79536033	0.01928622
H	1.	-2.79197189	-0.79536030	0.01928622
O	8.	-0.08681609	-0.00000019	-0.01204576
H	1.	1.76192036	-0.00000030	0.11462668
H	1.	-2.78079911	0.79536075	0.03875398
H	1.	-2.78078655	-0.79535988	0.03875397
O	8.	-0.11704140	-0.00000014	-0.01803717
H	1.	1.73554689	-0.00000027	0.17147140
H	1.	-2.76565999	0.79536065	0.05868983
H	1.	-2.76565027	-0.79535998	0.05868978
O	8.	-0.15815147	-0.00000218	-0.02400711
H	1.	1.70099691	-0.00000273	0.22784413
H	1.	-2.75047964	0.79536410	0.07944633
H	1.	-2.75037723	-0.79535653	0.07944410
O	8.	-0.20958947	-0.00001149	-0.02999142
H	1.	1.65984555	-0.00000974	0.28376592
H	1.	-2.73927824	0.79537656	0.10136564
H	1.	-2.73887413	-0.79534402	0.10134886

O	8.	-0.27178759	0.00000791	-0.03614945
H	1.	1.61487737	0.00000275	0.33964535
H	1.	-2.73564265	0.79535159	0.12468894
H	1.	-2.73583692	-0.79536903	0.12470573
O	8.	-0.34480381	0.00000671	-0.04267745
H	1.	1.56746778	0.00000032	0.39610473
H	1.	-2.74348168	0.79535446	0.14933790
H	1.	-2.74359810	-0.79536617	0.14935295
O	8.	-0.41566499	-0.00000081	-0.05029568
H	1.	1.54628569	0.00000722	0.45451901
H	1.	-2.75207467	0.79537448	0.17757827
H	1.	-2.75195551	-0.79534615	0.17757692

**Path between planar  $D_{3h}$  MEX to the out-of-plane  $C_{3v}$  MEX**

**Table SVa**

O	8.0	-0.00864699	0.01361791	0.00000000
H	1.0	1.83288945	-0.04085372	0.00000000
H	1.0	-0.92936306	-0.04085373	1.59481769
H	1.0	-0.92936306	-0.04085373	-1.59481769
O	8.0	-0.00863968	0.02731991	0.00000000
H	1.0	1.83322771	-0.08192940	0.00000000
H	1.0	-0.92946838	-0.08192752	1.59510388
H	1.0	-0.92946838	-0.08192752	-1.59510388
O	8.0	-0.00875673	0.04115770	0.00000000
H	1.0	1.83177533	-0.12332672	0.00000000
H	1.0	-0.92886556	-0.12330647	1.59394833
H	1.0	-0.92886556	-0.12330647	-1.59394833
O	8.0	-0.00899578	0.05518361	0.00000000
H	1.0	1.82847198	-0.16514206	0.00000000
H	1.0	-0.92752371	-0.16507249	1.59129877
H	1.0	-0.92752371	-0.16507249	-1.59129877
O	8.0	-0.00935182	0.06945082	0.00000000
H	1.0	1.82323686	-0.20746598	0.00000000
H	1.0	-0.92539952	-0.20730222	1.58708398
H	1.0	-0.92539952	-0.20730222	-1.58708398
O	8.0	-0.00981667	0.08401354	0.00000000
H	1.0	1.81596899	-0.25038031	0.00000000
H	1.0	-0.92243650	-0.25006469	1.58121345
H	1.0	-0.92243650	-0.25006469	-1.58121345
O	8.0	-0.01037827	0.09892710	0.00000000
H	1.0	1.80654771	-0.29395466	0.00000000
H	1.0	-0.91856410	-0.29341881	1.57357726

H	1.0	-0.91856410	-0.29341881	-1.57357726
O	8.0	-0.01101994	0.11424791	0.00000000
H	1.0	1.79483374	-0.33824233	0.00000000
H	1.0	-0.91369661	-0.33741055	1.56404593
H	1.0	-0.91369661	-0.33741055	-1.56404593
O	8.0	-0.01171954	0.13003332	0.00000000
H	1.0	1.78067077	-0.38327557	0.00000000
H	1.0	-0.90773184	-0.38206997	1.55247071
H	1.0	-0.90773184	-0.38206997	-1.55247071
O	8.0	-0.01244856	0.14634119	0.00000000
H	1.0	1.76388802	-0.42906025	0.00000000
H	1.0	-0.90054982	-0.42740800	1.53868420
H	1.0	-0.90054982	-0.42740800	-1.53868420