Supplementary tables for the article (C002193H)

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The results of Ar-OH in Tables S1 – S6 are given for comparison, which have been newly obtained by the reanalysis based on the new *ab initio* potential surface at the UCCSD(T)/aug-cc-pV5Z level of theory. Experimental data utilized in the reanalysis are exactly the same as those in our previous analysis, *Journal of Chemical Physics*, 2006, **125**, 124307.

Table S1. FTMW data of Ar-OH [a]

v_s'	v'	J'	F'	P'	v_s''	v''	J''	F''	P''	parity	Obs.	O – C [b]
0	0	2.5	2.0	1.5	0	0	1.5	1.0	1.5	–	15349.305	0.003
0	0	2.5	3.0	1.5	0	0	1.5	2.0	1.5	–	15336.420	0.003
0	0	2.5	2.0	1.5	0	0	1.5	2.0	1.5	–	15310.581	0.005
0	0	2.5	2.0	1.5	0	0	1.5	1.0	1.5	+	15364.495	–0.002
0	0	2.5	3.0	1.5	0	0	1.5	2.0	1.5	+	15351.583	–0.003
0	0	2.5	2.0	1.5	0	0	1.5	2.0	1.5	+	15325.777	–0.012
0	0	3.5	3.0	1.5	0	0	2.5	2.0	1.5	–	21499.253	–0.008
0	0	3.5	4.0	1.5	0	0	2.5	3.0	1.5	–	21493.518	–0.013
0	0	3.5	3.0	1.5	0	0	2.5	2.0	1.5	+	21469.644	–0.003
0	0	3.5	4.0	1.5	0	0	2.5	3.0	1.5	+	21463.955	0.002
0	0	4.5	4.0	1.5	0	0	3.5	3.0	1.5	–	27585.573	0.005
0	0	4.5	5.0	1.5	0	0	3.5	4.0	1.5	–	27582.483	0.005
0	0	4.5	4.0	1.5	0	0	3.5	3.0	1.5	+	27633.258	–0.007
0	0	4.5	5.0	1.5	0	0	3.5	4.0	1.5	+	27630.127	–0.004
0	0	5.5	5.0	1.5	0	0	4.5	4.0	1.5	–	33761.596	0.001
0	0	5.5	6.0	1.5	0	0	4.5	5.0	1.5	–	33759.695	–0.005
0	0	5.5	5.0	1.5	0	0	4.5	4.0	1.5	+	33693.035	0.003
0	0	5.5	6.0	1.5	0	0	4.5	5.0	1.5	+	33691.184	–0.003
0	0	6.5	6.0	1.5	0	0	5.5	5.0	1.5	–	39790.012	–0.006
0	0	6.5	7.0	1.5	0	0	5.5	6.0	1.5	–	39788.864	–0.002
0	0	6.5	6.0	1.5	0	0	5.5	5.0	1.5	+	39881.260	0.020
0	0	6.5	7.0	1.5	0	0	5.5	6.0	1.5	+	39880.052	0.019
0	0	7.5	7.0	1.5	0	0	6.5	6.0	1.5	–	45989.467	–0.017
0	0	7.5	8.0	1.5	0	0	6.5	7.0	1.5	–	45988.700	0.003
0	0	7.5	7.0	1.5	0	0	6.5	6.0	1.5	+	45874.859	0.009
0	0	7.5	8.0	1.5	0	0	6.5	7.0	1.5	+	45874.115	–0.006
1	0	2.5	2.0	1.5	1	0	1.5	1.0	1.5	–	15135.140	0.000
1	0	2.5	3.0	1.5	1	0	1.5	2.0	1.5	–	15123.433	–0.004
1	0	2.5	2.0	1.5	1	0	1.5	2.0	1.5	–	15100.037	0.013
1	0	2.5	2.0	1.5	1	0	1.5	1.0	1.5	+	15149.777	–0.008
1	0	2.5	3.0	1.5	1	0	1.5	2.0	1.5	+	15138.052	–0.007
1	0	2.5	2.0	1.5	1	0	1.5	2.0	1.5	+	15114.685	0.002

Table S1 Continued [a]

v_s'	v'	J'	F'	P'	v_s''	v''	J''	F''	P''	parity	Obs.	O – C [b]
1	0	3.5	3.0	1.5	1	0	2.5	2.0	1.5	–	21199.744	–0.003
1	0	3.5	4.0	1.5	1	0	2.5	3.0	1.5	–	21194.533	–0.003
1	0	3.5	3.0	1.5	1	0	2.5	2.0	1.5	+	21171.280	0.001
1	0	3.5	4.0	1.5	1	0	2.5	3.0	1.5	+	21166.102	0.004
1	0	4.5	4.0	1.5	1	0	3.5	3.0	1.5	–	27203.229	0.010
1	0	4.5	5.0	1.5	1	0	3.5	4.0	1.5	–	27200.386	–0.013
1	0	4.5	4.0	1.5	1	0	3.5	3.0	1.5	+	27248.930	0.018
1	0	4.5	5.0	1.5	1	0	3.5	4.0	1.5	+	27246.044	–0.012
2	0	2.5	2.0	1.5	2	0	1.5	1.0	1.5	–	14897.631	0.010
2	0	2.5	3.0	1.5	2	0	1.5	2.0	1.5	–	14887.249	0.003
2	0	2.5	2.0	1.5	2	0	1.5	1.0	1.5	+	14912.673	–0.001
2	0	2.5	3.0	1.5	2	0	1.5	2.0	1.5	+	14902.272	–0.008
2	0	3.5	3.0	1.5	2	0	2.5	2.0	1.5	–	20869.325	0.016
2	0	3.5	4.0	1.5	2	0	2.5	3.0	1.5	–	20864.678	–0.011
2	0	3.5	3.0	1.5	2	0	2.5	2.0	1.5	+	20840.153	–0.001
2	0	3.5	4.0	1.5	2	0	2.5	3.0	1.5	+	20835.552	–0.007

[a] In MHz.

[b] Observed minus calculated frequencies.

Table S2. FTMW data of Ar-OD [a]

v_s'	v'	J'	F'	P'	v_s''	v''	J''	F''	P''	parity	Obs.	O – C [b]
0	0	2.5	1.5	1.5	0	0	1.5	0.5	1.5	–	15014.943	0.007
0	0	2.5	2.5	1.5	0	0	1.5	1.5	1.5	–	15013.551	0.003
0	0	2.5	3.5	1.5	0	0	1.5	2.5	1.5	–	15010.020	0.008
0	0	2.5	1.5	1.5	0	0	1.5	1.5	1.5	–	15009.489	0.005
0	0	2.5	2.5	1.5	0	0	1.5	2.5	1.5	–	15004.347	0.003
0	0	2.5	1.5	1.5	0	0	1.5	0.5	1.5	+	15021.848	0.005
0	0	2.5	2.5	1.5	0	0	1.5	1.5	1.5	+	15020.454	0.000
0	0	2.5	3.5	1.5	0	0	1.5	2.5	1.5	+	15016.915	–0.004
0	0	2.5	1.5	1.5	0	0	1.5	1.5	1.5	+	15016.398	0.004
0	0	2.5	2.5	1.5	0	0	1.5	2.5	1.5	+	15011.252	–0.001
0	0	3.5	2.5	1.5	0	0	2.5	1.5	1.5	–	21023.351	0.002
0	0	3.5	3.5	1.5	0	0	2.5	2.5	1.5	–	21022.607	0.013
0	0	3.5	4.5	1.5	0	0	2.5	3.5	1.5	–	21021.123	–0.006
0	0	3.5	2.5	1.5	0	0	2.5	1.5	1.5	+	21009.828	0.012
0	0	3.5	3.5	1.5	0	0	2.5	2.5	1.5	+	21009.076	0.013
0	0	3.5	4.5	1.5	0	0	2.5	3.5	1.5	+	21007.612	0.012
0	0	4.5	3.5	1.5	0	0	3.5	2.5	1.5	–	26999.319	–0.009
0	0	4.5	4.5	1.5	0	0	3.5	3.5	1.5	–	26998.875	–0.001
0	0	4.5	5.5	1.5	0	0	3.5	4.5	1.5	–	26998.090	–0.011
0	0	4.5	3.5	1.5	0	0	3.5	2.5	1.5	+	27021.262	–0.004
0	0	4.5	4.5	1.5	0	0	3.5	3.5	1.5	+	27020.828	0.017
0	0	4.5	5.5	1.5	0	0	3.5	4.5	1.5	+	27020.027	–0.008
0	0	5.5	4.5	1.5	0	0	4.5	3.5	1.5	–	33012.691	–0.008
0	0	5.5	5.5	1.5	0	0	4.5	4.5	1.5	–	33012.395	–0.012
0	0	5.5	6.5	1.5	0	0	4.5	5.5	1.5	–	33011.930	–0.011
0	0	5.5	4.5	1.5	0	0	4.5	3.5	1.5	+	32980.913	0.003
0	0	5.5	5.5	1.5	0	0	4.5	4.5	1.5	+	32980.624	0.003
0	0	5.5	6.5	1.5	0	0	4.5	5.5	1.5	+	32980.144	–0.014
0	0	6.5	5.5	1.5	0	0	5.5	4.5	1.5	–	38952.701	–0.002
0	0	6.5	6.5	1.5	0	0	5.5	5.5	1.5	–	38952.510	–0.002
0	0	6.5	7.5	1.5	0	0	5.5	6.5	1.5	–	38952.213	–0.003
0	0	6.5	5.5	1.5	0	0	5.5	4.5	1.5	+	38995.422	0.014
0	0	6.5	6.5	1.5	0	0	5.5	5.5	1.5	+	38995.217	0.004
0	0	6.5	7.5	1.5	0	0	5.5	6.5	1.5	+	38994.909	–0.005

[a] In MHz.

[b] Observed minus calculated frequencies.

Table S3. IR-UV double resonance data of Ar-OH [a]

v_s'	v'	J'	P'	v_s''	v''	J''	P''	parity	Obs.	O – C [b]
1	0	6.5	1.5	0	0	7.5	1.5	+/– [c]	3566.22	–0.02
1	0	5.5	1.5	0	0	6.5	1.5	+/– [c]	3566.45	–0.01
1	0	4.5	1.5	0	0	5.5	1.5	+/– [c]	3566.67	–0.01
1	0	3.5	1.5	0	0	4.5	1.5	+/– [c]	3566.90	0.00
1	0	2.5	1.5	0	0	3.5	1.5	+/– [c]	3567.12	0.01
1	0	1.5	1.5	0	0	2.5	1.5	+/– [c]	3567.34	0.02
1	0	1.5	1.5	0	0	1.5	1.5	+/– [c]	3567.83	0.00
1	0	2.5	1.5	0	0	1.5	1.5	+/– [c]	3568.35	0.01
1	0	3.5	1.5	0	0	2.5	1.5	+/– [c]	3568.54	0.01
1	0	4.5	1.5	0	0	3.5	1.5	+/– [c]	3568.73	0.00
1	0	5.5	1.5	0	0	4.5	1.5	+/– [c]	3568.92	0.01
1	0	6.5	1.5	0	0	5.5	1.5	+/– [c]	3569.12	0.02
1	0	7.5	1.5	0	0	6.5	1.5	+/– [c]	3569.29	0.01
1	0	2.5	0.5	0	0	3.5	1.5	+	3576.87	–0.02
1	0	2.5	0.5	0	0	3.5	1.5	–	3575.81	–0.03
1	0	1.5	0.5	0	0	2.5	1.5	+	3576.16	–0.01
1	0	1.5	0.5	0	0	2.5	1.5	–	3576.87	0.00
1	0	0.5	0.5	0	0	1.5	1.5	+	3576.87	0.00
1	0	0.5	0.5	0	0	1.5	1.5	–	3576.51	–0.02
1	0	1.5	0.5	0	0	1.5	1.5	+	3576.68	0.00
1	0	1.5	0.5	0	0	1.5	1.5	–	3577.37	–0.01
1	0	2.5	0.5	0	0	2.5	1.5	+	3577.59	–0.01
1	0	2.5	0.5	0	0	2.5	1.5	–	3576.54	–0.02
1	0	3.5	0.5	0	0	3.5	1.5	+	3576.51	0.06 [d]
1	0	3.5	0.5	0	0	3.5	1.5	–	3577.84	0.00 [d]
1	0	2.5	0.5	0	0	1.5	1.5	+	3578.09	–0.03 [d]
1	0	2.5	0.5	0	0	1.5	1.5	–	3577.11	0.04 [d]
1	0	3.5	0.5	0	0	2.5	1.5	+	3577.17	0.00 [d]
1	0	3.5	0.5	0	0	2.5	1.5	–	3578.54	–0.02 [d]
1	0	4.5	0.5	0	0	3.5	1.5	+	3579.01	0.00 [d]
2	0	1.5	1.5	0	0	1.5	1.5	+/– [c]	6970.4	–0.24

[a] In cm^{-1}.

[b] Observed minus calculated frequencies.

[c] Not resolved.

[d] Not included in the analysis.

Table S4. SEP data of Ar-OH [a]

v_s'	v'	J'	P'	v_s''	v''	J''	P''	parity	Obs.	O – C [b]
0	0	1.5	0.5	0	0	1.5	1.5	- [c]	9.19	–0.23
0	0	1.5	–0.5	0	0	1.5	1.5	- [c]	19.2	–0.5
0	0	1.5	–1.5	0	0	1.5	1.5	- [c]	21.3	0.0
0	1	1.5	1.5	0	0	1.5	1.5	- [c]	34.9	0.3

[a] In cm^{-1}.

[b] Observed minus calculated frequencies.

[c] Parity components were not resolved.

Table S5 3D average potential parameters of Ar–OH [a]

	q^0 Fitted	q^0 *ab initio*		q^1 Fitted	q^1 *ab initio*		q^2 Fitted	q^2 *ab initio*
$b^0_{\Pi e}$/Å^{-1}	→ [b]	–3.4435	$b^0_{\Pi 1}$/Å^{-2}	→	0.8021	$b^0_{\Pi 2}$/Å^{-3}	→	0.4879
$b^1_{\Pi e}$/Å^{-1}	→	0.6201	$b^1_{\Pi 1}$/Å^{-2}	→	0.1137	$b^1_{\Pi 2}$/Å^{-3}	→	–0.00305
$b^2_{\Pi e}$/Å^{-1}	→	0.00246	$b^2_{\Pi 1}$/Å^{-2}	→	–0.0145	$b^2_{\Pi 2}$/Å^{-3}	→	–0.1996
$g^0_{0,\Pi e}$/cm^{-1}	$-7.905(34)\times10^6$	-7.5551×10^6	$g^0_{0,\Pi 1}$/cm^{-1}Å^{-1}	$6.544(28)\times10^7$	6.0510×10^7	$g^0_{0,\Pi 2}$/cm^{-1}Å^{-2}	$-2.423(16)\times10^8$	-2.1312×10^8
$g^1_{0,\Pi e}$/cm^{-1}	$5.9417(77)\times10^7$	5.9089×10^7	$g^1_{0,\Pi 1}$/cm^{-1}Å^{-1}	$-1.4995(28)\times10^8$	-1.4495×10^8	$g^1_{0,\Pi 2}$/cm^{-1}Å^{-2}	$3.067(17)\times10^8$	2.7786×10^8
$g^2_{0,\Pi e}$/cm^{-1}	$-3.0649(45)\times10^7$	-3.0654×10^7	$g^2_{0,\Pi 1}$/cm^{-1}Å^{-1}	→	5.7487×10^7	$g^2_{0,\Pi 2}$/cm^{-1}Å^{-2}	→	-1.7152×10^8
$g^3_{0,\Pi e}$/cm^{-1}	→	1.8032×10^7	$g^3_{0,\Pi 1}$/cm^{-1}Å^{-1}	→	-2.9275×10^6			
$g^4_{0,\Pi e}$/cm^{-1}	→	1.5523×10^6						

Table S5 Continued [a]

q⁰			q¹			q²		
	Fitted	*ab initio*		Fitted	*ab initio*		Fitted	*ab initio*
$g^{0}_{1,\Pi e}$ /cm^{-1}Å^{-1}	→	2.3539×10^{7}	$g^{0}_{1,\Pi 1}$ /cm^{-1}Å^{-2}	→	-5.5447×10^{7}	$g^{0}_{1,\Pi 2}$ /cm^{-1}Å^{-3}	→	1.0862×10^{8}
$g^{1}_{1,\Pi e}$ /cm^{-1}Å^{-1}	→	-5.5906×10^{7}	$g^{1}_{1,\Pi 1}$ /cm^{-1}Å^{-2}	→	1.0444×10^{8}	$g^{1}_{1,\Pi 2}$ /cm^{-1}Å^{-3}	→	-1.4500×10^{8}
$g^{2}_{1,\Pi e}$ /cm^{-1}Å^{-1}	→	3.0720×10^{7}	$g^{2}_{1,\Pi 1}$ /cm^{-1}Å^{-2}	→	-3.6302×10^{7}	$g^{2}_{1,\Pi 2}$ /cm^{-1}Å^{-3}	→	7.0575×10^{7}
$g^{3}_{1,\Pi e}$ /cm^{-1}Å^{-1}	→	-1.3643×10^{7}	$g^{3}_{1,\Pi 1}$ /cm^{-1}Å^{-2}	→	4.6281×10^{6}			
$g^{0}_{2,\Pi e}$ /cm^{-1}Å^{-2}	→	-6.6451×10^{6}	$g^{0}_{2,\Pi 1}$ /cm^{-1}Å^{-3}	→	6.6665×10^{6}			
$g^{1}_{2,\Pi e}$ /cm^{-1}Å^{-2}	→	1.2638×10^{7}	$g^{1}_{2,\Pi 1}$ /cm^{-1}Å^{-3}	→	-1.2047×10^{7}			
$g^{2}_{2,\Pi e}$ /cm^{-1}Å^{-2}	→	-6.6026×10^{6}						
$g^{3}_{2,\Pi e}$ /cm^{-1}Å^{-2}	→	1.2047×10^{7}						

Table S5 Continued [a]

	q⁰ Fitted	q⁰ ab initio		q¹ Fitted	q¹ ab initio		q² Fitted	q² ab initio
$C^{0}_{6,\Pi e}$/cm^{-1}Å^{6}	–2.2715(78)×10^{5}	–2.2482×10^{5}	$C^{0}_{6,\Pi 1}$/ cm^{-1}Å^{5}	–3.3927(88)×10^{5}	–2.7261×10^{5}	$C^{0}_{6,\Pi 2}$/ cm^{-1}Å^{4}	→	2.7171×10^{5}
$C^{1}_{6,\Pi e}$/cm^{-1}Å^{6}	–5.631(99)×10^{4}	–5.4869×10^{4}	$C^{1}_{6,\Pi 1}$/ cm^{-1}Å^{5}	→	–2.4872×10^{5}	$C^{1}_{6,\Pi 2}$/ cm^{-1}Å^{4}	→	1.5836×10^{5}
$C^{2}_{6,\Pi e}$/cm^{-1}Å^{6}	–8.004(71)×10^{4}	–7.7254×10^{4}	$C^{2}_{6,\Pi 1}$/ cm^{-1}Å^{5}	→	–1.0151×10^{5}			
$C^{3}_{6,\Pi e}$/cm^{-1}Å^{6}	→	–2.2878×10^{4}	$C^{3}_{6,\Pi 1}$/ cm^{-1}Å^{5}	→	–3.5245×10^{4}			
$C^{4}_{6,\Pi e}$/cm^{-1}Å^{6}	→	–6.9243×10^{3}						
$C^{0}_{8,\Pi e}$/cm^{-1}Å^{8}	→	–1.8844×10^{6}	$C^{0}_{8,\Pi 1}$/ cm^{-1}Å^{7}	→	2.8819×10^{6}			
$C^{1}_{8,\Pi e}$/cm^{-1}Å^{8}	→	3.4307×10^{5}	$C^{1}_{8,\Pi 1}$/ cm^{-1}Å^{7}	→	3.4960×10^{6}			
$C^{2}_{8,\Pi e}$/cm^{-1}Å^{8}	→	7.1442×10^{5}						
		σ_{fit} /kHz		11.3				

[a]Values in parentheses denote one standard deviation of the fit and apply to the last digits.

[b]Fixed to the values from the *ab initio* calculation.

Table S6 3D difference potential parameters of Ar–OH [a]

	q^0			q^1			q^2	
	Fitted	*ab initio*		Fitted	*ab initio*		Fitted	*ab initio*
b_{2e}^{0} /Å^{-1}	→ [b]	–2.7343	b_{21}^{0} /Å^{-2}	→	0.1403	b_{22}^{0} /Å^{-3}	→	0.2092
b_{2e}^{1} /Å^{-1}	→	0.2329	b_{21}^{1} /Å^{-2}	→	–0.1085			
b_{2e}^{2} /Å^{-1}	→	0.0453	b_{21}^{2} /Å^{-2}	→				
b_{2e}^{3} /Å^{-1}	→	0.00502	b_{21}^{3} /Å^{-2}	→				
$g_{0,2e}^{0}$ /cm^{-1}	$4.2414(30)\times10^{6}$	4.2266×10^{6}	$g_{0,21}^{0}$ /cm^{-1}Å^{-1}	$-0.457(161)\times10^{6}$	-1.5094×10^{6}	$g_{0,22}^{0}$ /cm^{-1}Å^{-2}	$-10.07(92)\times10^{6}$	-1.9210×10^{6}
$g_{0,2e}^{1}$ /cm^{-1}	$-10.557(177)\times10^{5}$	-9.885×10^{5}	$g_{0,21}^{1}$ /cm^{-1}Å^{-1}	→	1.0074×10^{5}			
$g_{0,2e}^{2}$ /cm^{-1}	$12.2(26)\times10^{4}$	5.38×10^{4}	$g_{0,21}^{2}$ /cm^{-1}Å^{-1}	→				
$g_{1,2e}^{0}$ /cm^{-1}Å^{-1}	→	-9.4505×10^{5}	$g_{1,21}^{0}$ /cm^{-1}Å^{-2}	→	3.9408×10^{5}			
$g_{1,2e}^{1}$ /cm^{-1}Å^{-1}	→	2.0459×10^{5}	$g_{1,21}^{1}$ /cm^{-1}Å^{-2}	→	3.1993×10^{4}			
$C_{6,2e}^{0}$ /cm^{-1}Å^{6}	→	-2.2649×10^{4}	$C_{6,21}^{0}$ / cm^{-1}Å^{5}	→	-2.6511×10^{4}	$C_{6,22}^{6}$ / cm^{-1}Å^{4}	→	1.1638×10^{5}
$C_{6,2e}^{1}$ /cm^{-1}Å^{6}	→	1.1032×10^{4}	$C_{6,21}^{0}$ / cm^{-1}Å^{5}	→	-7.3600×10^{3}			
$C_{6,2e}^{2}$ /cm^{-1}Å^{6}	→	1.9673×10^{3}						

[a] Values in parentheses denote one standard deviation of the fit and apply to the last digits.

[b] Fixed to the values from the *ab initio* calculation