

Supporting Information

Table S1.

Species	GA (MP2/6-311++G(3df,3pd))	GA (M06-2X/6-311++G(3df,3pd))
H ₂ SeO	335.3954	333.5129
H ₂ SeO ₂	343.3647	347.1924
H ₂ SeO ₃	322.2178	326.4848
H ₂ SeO ₄	302.075	303.581
H ₂ SeO ₅	295.2352	296.4274
H ₂ Se ₂ O	320.7118	319.1431
H ₂ Se ₂ O ₃	289.5250	288.0189
H ₂ Se ₂ O ₄	329.3714	325.0416
H ₂ Se ₂ O ₆	277.9789	278.3554
H ₂ Se ₂ O ₇	280.6144	282.1831

Table S2.

Species	Total Energy			Free Energy		
	Neutral	Monoanion	Dianion	Neutral	Monoanion	Dianion
H ₂ SeO	-2476.2429	-2475.6902	-2474.9023	-2476.2469	-2475.7024	-2474.9236
H ₂ SeO ₂	-2551.3699	-2550.7992	-2550.0298	-2551.3688	-2550.8116	-2550.0524
H ₂ SeO ₃	-2626.4929	-2625.9580	-2625.2115	-2626.4921	-2625.9686	-2625.2312
H ₂ SeO ₄	-2701.5640	-2701.0605	-2700.3502	-2701.5587	-2701.0673	-2700.3676
H ₂ SeO ₅	-2776.5744	-2776.0831	-2775.3453	-2776.5680	-2776.0875	-2775.3640
H ₂ Se ₂ O	-4876.2226	-4875.6923	-4874.9336	-4876.2298	-4875.7087	-4874.9597
H ₂ Se ₂ O ₃	-5026.3953	-5025.9139	-5025.2291	-5026.3988	-5025.9274	-5025.2498
H ₂ Se ₂ O ₄	-5101.5538	-5101.0079	-5100.3285	-5101.5521	-5101.0172	-5100.3514
H ₂ Se ₂ O ₆	-5251.6690	-5251.2053	-5250.5557	-5251.6635	-5251.2105	-5250.5712
H ₂ Se ₂ O ₇	-5326.8084	-5326.3388	-5325.6927	-5326.7969	-5326.3397	-5325.7052

Table S3.

Species	Total Energy			Free Energy		
	Neutral	Monoanion	Dianion	Neutral	Monoanion	Dianion
H ₂ SeO	-2477.9493	-2477.3995	-2476.6050	-2477.9530	-2477.4115	-2476.6263
H ₂ SeO ₂	-2553.1762	-2552.5989	-2551.8248	-2553.1742	-2552.6109	-2551.8472
H ₂ SeO ₃	-2628.3883	-2627.8465	-2627.0948	-2628.3864	-2627.8561	-2627.1143
H ₂ SeO ₄	-2703.5555	-2703.0495	-2702.3365	-2703.5494	-2703.0556	-2702.3538
H ₂ SeO ₅	-2778.6715	-2778.1780	-2777.4408	-2778.6637	-2778.1813	-2777.4591
H ₂ Se ₂ O	-4879.5316	-4879.0043	-4878.2438	-4879.5384	-4879.0198	-4878.2697
H ₂ Se ₂ O ₃	-5029.8860	-5029.4091	-5028.7219	-5029.8887	-5029.4197	-5028.7425
H ₂ Se ₂ O ₄	-5105.1358	-5104.5968	-5103.9029	-5105.1337	-5104.6057	-5103.9257
H ₂ Se ₂ O ₆	-5255.4372	-5254.9726	-5254.3221	-5255.4305	-5254.9769	-5254.3374
H ₂ Se ₂ O ₇	-5330.6835	-5330.2107	-5329.5632	-5330.6709	-5330.2112	-5329.5753

Table S4.

Species	$\Delta G_{\text{sol.}}$		
	Neutral	Monoanion	Dianion
H ₂ SeO	-5.57	-65.11	-242.26
H ₂ SeO ₂	-9.14	-65.99	-241.34
H ₂ SeO ₃	-13.96	-63.33	-235.75
H ₂ SeO ₄	-15.76	-63.40	-224.48
H ₂ SeO ₅	-14.54	-60.75	-218.79
H ₂ Se ₂ O	-5.48	-56.30	-201.53
H ₂ Se ₂ O ₃	-16.32	-54.40	-203.07
H ₂ Se ₂ O ₄	-15.90	-62.99	-199.82
H ₂ Se ₂ O ₆	-22.33	-54.48	-185.97
H ₂ Se ₂ O ₇	-20.40	-50.16	-183.64

Table S5.

Species	$\Delta G_{\text{sol.}}$		
	Neutral	Monoanion	Dianion
H ₂ SeO	-6.80	-67.62	-251.08
H ₂ SeO ₂	-10.83	-71.72	-252.18
H ₂ SeO ₃	-18.77	-70.98	-248.93
H ₂ SeO ₄	-22.51	-70.22	-233.32
H ₂ SeO ₅	-21.12	-66.99	-225.08
H ₂ Se ₂ O	-6.55	-59.39	-209.24
H ₂ Se ₂ O ₃	-25.38	-60.82	-211.75
H ₂ Se ₂ O ₄	-24.85	-71.94	-214.50
H ₂ Se ₂ O ₆	-37.07	-67.49	-197.55
H ₂ Se ₂ O ₇	-32.46	-60.22	-194.43

Table S6.

Species	ΔG_g	$\Delta \Delta G_{sol}$	ΔG_{aq}	pK _a 1
H ₂ SeO	335.3954	-324.15	13.1354	9.66
H ₂ SeO ₂	343.3647	-321.46	21.9047	16.12
H ₂ SeO ₃	322.2178	-313.98	8.2378	6.06
H ₂ SeO ₄	302.0750	-312.25	-8.2850	-6.09
H ₂ SeO ₅	295.2352	-310.82	-13.6948	-10.07
H ₂ Se ₂ O	320.7118	-315.43	7.1718	5.27
H ₂ Se ₂ O ₃	289.5250	-302.69	-13.165	-9.68
H ₂ Se ₂ O ₄	329.3714	-311.70	19.5614	14.38
H ₂ Se ₂ O ₆	277.9789	-296.76	-16.8911	-12.42
H ₂ Se ₂ O ₇	280.6144	-294.37	-11.8656	-8.72

Table S7.

Species	ΔG_g	$\Delta\Delta G_{sol}$	ΔG_{aq}	pK _a 1
H ₂ SeO	333.5129	-325.43	9.9729	7.34
H ₂ SeO ₂	347.1924	-325.50	21.6924	15.96
H ₂ SeO ₃	326.4848	-316.82	9.6648	7.11
H ₂ SeO ₄	303.581	-312.32	-6.8490	-5.04
H ₂ SeO ₅	296.4274	-310.48	-12.1626	-8.95
H ₂ Se ₂ O	319.1431	-317.45	3.5831	2.63
H ₂ Se ₂ O ₃	288.0189	-300.05	-12.0311	-8.85
H ₂ Se ₂ O ₄	325.0416	-311.70	15.2316	11.21
H ₂ Se ₂ O ₆	278.3554	-295.03	-14.7846	-10.88
H ₂ Se ₂ O ₇	282.1831	-292.37	-8.2969	-6.10

Table S8.

Species	ΔG_g	$\Delta\Delta G_{sol}$	ΔG_{aq}	pK _{a2}
H ₂ SeO	482.4193	-441.76	42.5493	31.28
H ₂ SeO ₂	470.1203	-439.96	30.1603	22.19
H ₂ SeO ₃	456.4407	-437.03	19.4107	14.28
H ₂ SeO ₄	432.7838	-425.69	8.9838	6.60
H ₂ SeO ₅	447.7184	-422.65	26.9584	19.82
H ₂ Se ₂ O	463.7197	-409.84	55.7697	41.01
H ₂ Se ₂ O ₃	418.9160	-413.28	5.636	4.15
H ₂ Se ₂ O ₄	411.5115	-401.44	11.9615	8.79
H ₂ Se ₂ O ₆	394.8827	-396.10	0.6727	0.49
H ₂ Se ₂ O ₇	391.8707	-398.09	-4.3293	-3.18

Table S9.

Species	ΔG_g	$\Delta\Delta G_{sol}$	ΔG_{aq}	pK _{a2}
H ₂ SeO	486.4354	-448.07	40.2554	29.62
H ₂ SeO ₂	472.9440	-445.07	27.874	20.51
H ₂ SeO ₃	459.2017	-442.56	16.6417	12.24
H ₂ SeO ₄	434.1016	-427.71	8.2816	6.09
H ₂ SeO ₅	446.9027	-422.70	26.0927	19.20
H ₂ Se ₂ O	464.4100	-414.46	51.8400	38.14
H ₂ Se ₂ O ₃	418.6650	-415.54	3.125	2.30
H ₂ Se ₂ O ₄	420.4220	-407.17	15.1420	11.14
H ₂ Se ₂ O ₆	395.0082	-394.67	2.2282	1.64
H ₂ Se ₂ O ₇	392.7492	-398.82	-4.1808	-3.07

Molecular Cartesian Coordinates of Different Isomers of Some Oxoacids

HF/6-31G(d) Gas Phase

H₂SeO

Total Energy: -2473.5568927

H	0.591816	1.408086	-0.011370
O	-1.411195	0.015006	-0.114722
H	-1.761727	0.048832	0.765408
Se	0.366455	-0.046381	0.004816

Total Energy: -2473.5271824

H	-1.920872	0.769408	0.362623
O	-1.611513	-0.000006	-0.103992
H	-1.920895	-0.769361	0.362651
Se	0.492173	0.000000	0.003137

Total Energy: - 2473.5471173

H	-1.403338	-0.576906	0.000000
O	0.053328	1.429306	0.000000
H	-0.836442	1.755628	0.000000
Se	0.053328	-0.370975	0.000000

Total Energy: - 2473.4918292

H	-0.754326	-1.044852	0.880536
O	1.356868	-0.000047	0.064580
H	-0.753341	1.045716	0.879801
Se	-0.274920	-0.000014	-0.066970

H₂SeO₂

Total Energy: - 2548.4074343

O	0.000000	1.349515	-0.730232
O	0.000000	-1.349515	-0.730232
H	0.885738	1.493659	-1.039365

H	-0.885738	-1.493659	-1.039365
Se	0.000000	0.000000	0.404778

Total Energy: - 2548.404722

O	-1.357041	0.718545	-0.119793
O	1.357203	0.718423	-0.119803
H	-1.583455	1.047719	0.740223
H	1.583234	1.047839	0.740503
Se	-0.000032	-0.399744	0.012825

Total Energy: - 2548.358847

O	1.463184	0.448186	-0.028942
O	-1.165625	0.884802	0.026854
H	1.336203	1.323756	0.329323
H	-0.024557	-0.785582	1.370842
Se	-0.108592	-0.329473	-0.049514

Total Energy: - 2548.3421341

O	-2.039492	0.091568	-0.000038
O	0.928389	1.183243	-0.000006
H	-2.207432	0.634956	0.761412
H	-2.209067	0.635653	-0.760659
Se	0.391333	-0.337326	-0.000012

Total Energy: - 2548.2784477

O	1.124556	0.621379	-0.113635
O	2.059341	-0.409643	0.000578
H	1.284364	1.163902	0.654384
H	1.494514	-1.165740	0.163458
Se	-0.830884	-0.049766	0.002548

H₂SeO₃

Total Energy: - 2623.2405031

O	0.231403	-0.854282	1.318031
O	0.231403	-0.854282	-1.318031
H	-0.677350	-1.043801	1.543075
H	-0.677350	-1.043801	-1.543075
O	-1.276929	0.798751	0.000000
Se	0.231403	0.275473	0.000000

Total Energy: - 2623.2347766

O	-1.511401	-0.021955	0.448069
O	0.653849	1.417347	0.244306
H	-2.075538	0.607697	0.011156
H	0.958447	1.293780	1.141643
O	0.792703	-1.180087	0.569224
Se	0.048114	-0.106586	-0.330753

Total Energy: - 2623.1606259

O	-1.498739	-0.403642	-0.361726
O	1.057926	-1.175489	-0.153553
H	-0.072480	-0.023756	1.629911
H	1.819870	-0.780871	-0.572131
O	0.592506	1.416032	-0.296367
Se	-0.087086	0.062042	0.159864

Total Energy: - 2623.2066686

O	-0.476538	1.316227	0.584872
O	2.139063	-0.001421	-0.091828
H	2.288653	0.761416	0.456049
H	2.290952	-0.759886	0.461434
O	-0.479088	-1.315790	0.584673
Se	-0.413150	0.000187	-0.280565

Total Energy: - 2623.0363512

O		-0.965708	1.289821	1.113357
O		-0.965708	1.289821	-1.113357
H		-0.043707	1.294896	1.373991
H	0	-0.043707	1.294896	-1.373991
O		-0.965708	0.481412	0.000000
Se		0.684247	-0.796418	0.000000

Total Energy: - 2623.006289

O		-1.497950	-1.106302	0.129063
H		0.699587	0.529251	1.335832
H		-2.183057	-0.613986	0.585750
O		-1.529134	1.195044	0.076737
O		-0.830299	-0.017236	-0.436671
Se		0.951251	-0.014333	-0.002195

H₂SeO₅

Total Energy: - 2772.7831216

O		-0.053138	1.469137	0.716316
O		-1.507081	-0.136531	-1.047269
O		-0.425205	-1.099610	1.168988
O		1.092996	-0.343649	-0.862254
O		2.181788	-0.217889	-0.000200
H		-0.900800	-1.851464	0.821571
H		2.424508	0.698935	-0.101176
Se		-0.348194	0.111202	-0.015443

Total Energy: - 2772.731033

O		-0.187819	-0.966837	1.251267
O		1.709874	-0.452462	-0.602032
O		0.347037	1.472112	0.661214
O		-0.949071	-0.078908	-1.109216
O		-2.119832	0.107018	-0.109098
H		0.650568	2.135348	0.044028
H		-1.158241	-0.895377	1.229045
Se		0.297240	-0.055511	-0.059122

Total Energy: - 2772.7380101

O	-0.571836	-1.235989	-0.990054
O	-1.511945	0.251829	0.870175
O	-0.051386	1.495921	-0.682961
O	0.999046	-0.196405	1.186635
O	1.745924	-0.201179	-0.133457
H	0.840247	1.676697	-0.973676
H	-2.197587	-0.338736	0.569767
Se	-0.103561	-0.066217	-0.047023

Total Energy: - 2772.7050257

O	-0.266179	-1.371508	-0.913142
O	-1.563246	0.172407	0.984069
O	-0.153265	1.290322	-0.961834
O	1.074468	0.075103	0.930474
O	2.458661	0.044264	-0.060471
H	-0.509703	2.049830	-0.503811
H	1.204994	-0.686988	1.494084
Se	-0.385259	-0.089634	-0.024207

Total Energy: - 2772.7321177

O	-0.685648	1.550533	0.469479
O	1.445342	0.048579	0.619157
O	2.207978	-0.893480	-0.082271
O	-0.807336	-1.084261	0.374946
O	-2.127383	-0.995251	-0.078010
H	3.018658	-0.416698	-0.223948
H	-2.548662	-0.509836	0.625569
Se	-0.021577	0.350517	-0.318471

Total Energy: - 2772.4421095

O	0.957193	0.296301	1.507596
O	0.457823	1.994789	-0.437726
O	1.454835	-0.125921	-0.772573
O	1.663774	-1.376495	-0.305345
H	-1.392209	0.253877	-1.351656
H	2.083721	-1.214726	0.541310
Se	-1.207585	-0.270830	0.005867
O	0.512173	0.482462	0.084405

Total Energy: - 2772.4686824

O	-1.145099	0.774417	1.360214
O	-1.300871	-0.933819	-0.278054
O	-2.628600	-0.705881	-0.149658
H	-0.109764	1.139162	-1.487182
H	-2.718996	-0.512139	0.785647
O	-0.647993	0.265679	0.022185
O	-0.918781	1.180520	-0.971059
Se	1.645868	-0.155128	0.024486

Total Energy: - 2772.5336792

O	-1.129047	1.234290	-1.048875
O	1.516315	1.110802	0.277284
H	-2.273516	0.036579	1.181789
H	1.420291	1.647474	-0.505549
O	-0.954363	0.109311	-0.042902
O	-1.428413	0.490660	1.203788
Se	0.864480	-0.456596	-0.023691
O	-1.571879	-1.215038	-0.373140

Total Energy: - 2772.4322215

O	-1.016517	1.589129	0.164686
H	-2.119561	-1.061797	1.037260
H	1.580497	1.197341	-0.709401
O	-1.214380	0.078765	-0.011722
O	-1.341905	-0.526418	1.220114
O	-2.490543	-0.343165	-0.803633
O	-0.136636	-0.517794	-0.685228
Se	1.474674	-0.069991	0.017600

HSeO₅⁻

Total Energy: - 2772.2779302

Se	-0.377922	0.039483	0.033521
O	-0.660965	1.314631	-0.874091
O	-1.420173	-1.153242	-0.101481
O	0.127296	0.378061	1.518094
O	1.098840	-0.731351	-0.603750
O	2.209370	0.007745	-0.175443

H	2.014404	0.130816	0.753653
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Total Energy: - 2772.2146854

Se	-0.418067	-0.059048	0.016907
O	-0.255998	-0.780469	1.418006
O	-1.207077	1.324995	0.059671
O	-0.652202	-0.977959	-1.251342
O	1.242433	0.667426	-0.336876
O	2.486429	-0.164754	0.014381
H	1.305597	1.453722	0.194461

Total Energy: - 2772.2310769

Se	0.148371	0.071070	0.065783
O	0.403329	-0.745926	1.408230
O	1.561323	-0.398709	-0.852150
O	0.225832	1.652475	0.069637
O	-1.003469	-0.573689	-0.928651
O	-2.060658	-0.097120	0.067912
H	1.944511	-1.112633	-0.356428

Total Energy: - 2772.2779302

Se	-0.377854	0.039486	0.033624
O	-0.660857	1.316358	-0.871521
O	-1.420265	-1.152821	-0.103841
O	0.127417	0.374714	1.518938
O	1.098595	-0.730476	-0.605006
O	2.209167	0.008206	-0.175682
H	2.014601	0.129640	0.753669

Total Energy: - 2771.9930655

O	1.391071	0.676354	1.278866
O	1.476478	-1.239900	-0.277529
O	1.071294	1.059542	-1.115722
O	-1.458922	1.161490	0.107884
H	-0.941606	1.646233	-0.537296
O	0.949598	0.110528	-0.012959
Se	-0.779251	-0.464422	0.020382

Total Energy: - 2771.9017953

O	1.173925	-1.205014	0.833200
O	2.429802	0.043182	-0.820196
O	1.122783	1.181333	0.864749
O	0.168547	-0.014739	-0.859459
H	-1.586037	1.412861	0.007896
Se	-1.399704	-0.043742	-0.019028
O	1.251939	0.004532	0.061590

Total Energy: - 2771.9414374

O	-1.197345	-0.582829	1.406699
O	-0.885446	-1.699927	-0.745892
O	-1.431767	0.474891	-0.676217
O	-1.336453	1.673771	-0.041642
H	-0.409229	1.895024	-0.143510
O	-0.679749	-0.474498	0.053090
Se	1.313391	0.087462	0.005153