

SUPPORTING INFORMATION

Dependence of pK_a on Solute Cavity for Diprotic and Triprotic Acids

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Table S1. Point Group, DFT Method, Cavity Model, Total Energies (hartrees), Zero-point Energies (kcal/mol) with number of Imaginary Frequencies in Parentheses, Thermal Corrections (kcal/mol), Entropies (cal/mol·K), and Free energy of Solvation (kcal/mol)

	PG ^a	DFT	Cavity Model	SCF Energy	ZPE ^b (NIF)	TC ^c	S ^d	Solvation Free Energy ^e
CO ₃ ²⁻	D _{3h}	B3LYP	UFF	-263.79277	8.20 (0)	2.62	59.07	-264.00
HCO ₃ ⁻	C _s	B3LYP	UFF	-264.57336	16.28 (0)	2.82	63.70	-244.44
H ₂ CO ₃	C _{2v}	B3LYP	UFF	-265.12195	24.77 (0)	2.92	62.91	-63.63
CO ₃ ²⁻	D _{3h}	B3LYP	UAKS	-263.79277	8.20 (0)	2.62	59.07	-3.83
HCO ₃ ⁻	C _s	B3LYP	UAKS	-264.57336	16.28 (0)	2.82	63.70	-255.08
H ₂ CO ₃	C _{2v}	B3LYP	UAKS	-265.12195	24.77 (0)	2.92	62.91	-70.20
CO ₃ ²⁻	D _{3h}	B3LYP	Pauling	-263.79277	8.20 (0)	2.62	59.07	-12.01
HCO ₃ ⁻	C _s	B3LYP	Pauling	-264.57336	16.28 (0)	2.82	63.70	-262.91
H ₂ CO ₃	C _{2v}	B3LYP	Pauling	-265.12195	24.77 (0)	2.92	62.91	-73.01
CO ₃ ²⁻	D _{3h}	B3LYP	Klamt	-263.79277	8.20 (0)	2.62	59.07	-13.02
HCO ₃ ⁻	C _s	B3LYP	Klamt	-264.57336	16.28 (0)	2.82	63.70	-246.01
H ₂ CO ₃	C _{2v}	B3LYP	Klamt	-265.12195	24.77 (0)	2.92	62.91	-64.99
CO ₃ ²⁻	D _{3h}	B3LYP	SMD	-263.79277	8.20 (0)	2.62	59.07	-255.86
HCO ₃ ⁻	C _s	B3LYP	SMD	-264.57336	16.28 (0)	2.82	63.70	-68.48
H ₂ CO ₃	C _{2v}	B3LYP	SMD	-265.12195	24.77 (0)	2.92	62.91	-8.53
CO ₃ ²⁻	D _{3h}	PBE	UFF	-263.52597	7.77 (0)	2.66	59.32	-6.21
HCO ₃ ⁻	C _s	PBE	UFF	-264.30257	15.67 (0)	2.86	63.98	-241.50
H ₂ CO ₃	C _{2v}	PBE	UFF	-264.84861	24.01 (0)	2.96	63.15	-62.59
CO ₃ ²⁻	D _{3h}	PBE	UAKS	-263.52597	7.77 (0)	2.66	59.32	-3.43
HCO ₃ ⁻	C _s	PBE	UAKS	-264.30257	15.67 (0)	2.86	63.98	-251.73
H ₂ CO ₃	C _{2v}	PBE	UAKS	-264.84861	24.01 (0)	2.96	63.15	-68.79
CO ₃ ²⁻	D _{3h}	PBE	Pauling	-263.52597	7.77 (0)	2.66	59.32	-11.66
HCO ₃ ⁻	C _s	PBE	Pauling	-264.30257	15.67 (0)	2.86	63.98	-258.57
H ₂ CO ₃	C _{2v}	PBE	Pauling	-264.84861	24.01 (0)	2.96	63.15	-70.86
CO ₃ ²⁻	D _{3h}	PBE	Klamt	-263.52597	7.77 (0)	2.66	59.32	-12.42
HCO ₃ ⁻	C _s	PBE	Klamt	-264.30257	15.67 (0)	2.86	63.98	-242.96
H ₂ CO ₃	C _{2v}	PBE	Klamt	-264.84861	24.01 (0)	2.96	63.15	-63.91
CO ₃ ²⁻	D _{3h}	PBE	SMD	-263.52597	7.77 (0)	2.66	59.32	-252.26
HCO ₃ ⁻	C _s	PBE	SMD	-264.30257	15.67 (0)	2.86	63.98	-66.85
H ₂ CO ₃	C _{2v}	PBE	SMD	-264.84861	24.01 (0)	2.96	63.15	-7.94
CO ₃ ²⁻	D _{3h}	BVP86	UFF	-263.82022	7.75 (0)	2.66	59.32	-5.45
HCO ₃ ⁻	C _s	BVP86	UFF	-264.59765	15.62 (0)	2.87	64.01	-242.42
H ₂ CO ₃	C _{2v}	BVP86	UFF	-265.14436	23.96 (0)	2.96	63.16	-62.89
CO ₃ ²⁻	D _{3h}	BVP86	UAKS	-263.82022	7.75 (0)	2.66	59.32	-3.47
HCO ₃ ⁻	C _s	BVP86	UAKS	-264.59765	15.62 (0)	2.87	64.01	-252.79
H ₂ CO ₃	C _{2v}	BVP86	UAKS	-265.14436	23.96 (0)	2.96	63.16	-69.12
CO ₃ ²⁻	D _{3h}	BVP86	Pauling	-263.82022	7.75 (0)	2.66	59.32	-11.69
HCO ₃ ⁻	C _s	BVP86	Pauling	-264.59765	15.62 (0)	2.87	64.01	-259.87

H ₂ CO ₃	C _{2v}	BVP86	Pauling	-265.14436	23.96 (0)	2.96	63.16	-71.36
CO ₃ ²⁻	D _{3h}	BVP86	Klamt	-263.82022	7.75 (0)	2.66	59.32	-12.54
HCO ₃ ⁻	C _s	BVP86	Klamt	-264.59765	15.62 (0)	2.87	64.01	-243.91
H ₂ CO ₃	C _{2v}	BVP86	Klamt	-265.14436	23.96 (0)	2.96	63.16	-64.22
CO ₃ ²⁻	D _{3h}	BVP86	Klamt	-263.82022	7.75 (0)	2.66	59.32	-253.45
HCO ₃ ⁻	C _s	BVP86	Klamt	-264.59765	15.62 (0)	2.87	64.01	-67.29
H ₂ CO ₃	C _{2v}	BVP86	Klamt	-265.14436	23.96 (0)	2.96	63.16	-8.03
CO ₃ ²⁻	D _{3h}	M052X	UFF	-263.76479	8.63 (0)	2.59	58.91	-5.49
HCO ₃ ⁻	C _s	M052X	UFF	-264.54603	16.78 (0)	2.78	63.46	-248.54
H ₂ CO ₃	C _{2v}	M052X	UFF	-265.09311	25.25 (0)	2.89	62.72	-65.15
CO ₃ ²⁻	D _{3h}	M052X	UAKS	-263.76479	8.63 (0)	2.59	58.91	-4.33
HCO ₃ ⁻	C _s	M052X	UAKS	-264.54603	16.78 (0)	2.78	63.46	-259.86
H ₂ CO ₃	C _{2v}	M052X	UAKS	-265.09311	25.25 (0)	2.89	62.72	-71.75
CO ₃ ²⁻	D _{3h}	M052X	Pauling	-263.76479	8.63 (0)	2.59	58.91	-12.61
HCO ₃ ⁻	C _s	M052X	Pauling	-264.54603	16.78 (0)	2.78	63.46	-269.03
H ₂ CO ₃	C _{2v}	M052X	Pauling	-265.09311	25.25 (0)	2.89	62.72	-75.38
CO ₃ ²⁻	D _{3h}	M052X	Klamt	-263.76479	8.63 (0)	2.59	58.91	-14.07
HCO ₃ ⁻	C _s	M052X	Klamt	-264.54603	16.78 (0)	2.78	63.46	-250.18
H ₂ CO ₃	C _{2v}	M052X	Klmat	-265.09311	25.25 (0)	2.89	62.72	-66.61
CO ₃ ²⁻	D _{3h}	M052X	SMD	-263.76479	8.63 (0)	2.59	58.91	-261.00
HCO ₃ ⁻	C _s	M052X	SMD	-264.54603	16.78 (0)	2.78	63.46	-70.45
H ₂ CO ₃	C _{2v}	M052X	SMD	-265.09311	25.25 (0)	2.89	62.72	-9.09
SO ₃ ²⁻	C _{3v}	B3LYP	UFF	-623.89243	5.80 (0)	2.95	63.78	-231.27
HSO ₃ ⁻	C ₁	B3LYP	UFF	-624.64482	12.81 (0)	3.46	69.17	-59.68
H ₂ SO ₃	C _s	B3LYP	UFF	-625.17435	20.07 (0)	3.72	70.97	-4.27
SO ₃ ²⁻	C _{3v}	B3LYP	UAKS	-623.89243	5.80 (0)	2.95	63.78	-224.11
HSO ₃ ⁻	C ₁	B3LYP	UAKS	-624.64482	12.81 (0)	3.46	69.15	-56.26
H ₂ SO ₃	C _s	B3LYP	UAKS	-625.17435	20.07 (0)	3.72	70.97	-3.80
SO ₃ ²⁻	C _{3v}	B3LYP	Pauling	-623.89243	5.80 (0)	2.95	63.78	-246.74
HSO ₃ ⁻	C ₁	B3LYP	Pauling	-624.64482	12.81 (0)	3.46	69.17	-68.20
H ₂ SO ₃	C _s	B3LYP	Pauling	-625.17435	20.07 (0)	3.72	70.97	-12.91
SO ₃ ²⁻	C _{3v}	B3LYP	Klamt	-623.89243	5.80 (0)	2.95	63.78	-232.65
HSO ₃ ⁻	C ₁	B3LYP	Klamt	-624.64482	12.81 (0)	3.46	69.16	-60.74
H ₂ SO ₃	C _s	B3LYP	Klamt	-625.17435	20.07 (0)	3.72	70.97	-6.18
SO ₃ ²⁻	C _{3v}	B3LYP	SMD	-623.89243	5.80 (0)	2.95	63.78	-238.03
HSO ₃ ⁻	C ₁	B3LYP	SMD	-624.64482	12.81 (0)	3.46	69.16	-65.49
H ₂ SO ₃	C _s	B3LYP	SMD	-625.17435	20.07 (0)	3.72	70.97	-9.83
SO ₃ ²⁻	C _{3v}	PBE	UFF	-623.49623	5.48 (0)	3.02	64.21	-228.12
HSO ₃ ⁻	C ₁	PBE	UFF	-624.24488	12.28 (0)	3.53	69.63	-58.50
H ₂ SO ₃	C _s	PBE	UFF	-624.77117	19.30 (0)	3.82	71.77	-3.67
SO ₃ ²⁻	C _{3v}	PBE	UAKS	-623.49623	5.48 (0)	3.02	64.21	-221.46
HSO ₃ ⁻	C ₁	PBE	UAKS	-624.24488	12.28 (0)	3.53	69.65	-55.37
H ₂ SO ₃	C _s	PBE	UAKS	-624.77117	19.30 (0)	3.82	71.77	-3.24
SO ₃ ²⁻	C _{3v}	PBE	Pauling	-623.49623	5.48 (0)	3.02	64.21	-242.13
HSO ₃ ⁻	C ₁	PBE	Pauling	-624.24488	12.29 (0)	3.53	69.63	-65.77
H ₂ SO ₃	C _s	PBE	Pauling	-624.77117	19.30 (0)	3.82	71.77	-11.57
SO ₃ ²⁻	C _{3v}	PBE	Klamt	-623.49624	5.48 (0)	3.02	64.21	-229.40

HSO ₃ ⁻	C ₁	PBE	Klamt	-624.24488	12.29(0)	3.53	69.63	-59.52
H ₂ SO ₃	C _s	PBE	Klamt	-624.77117	19.30(0)	3.82	71.77	-5.48
SO ₃ ²⁻	C _{3v}	PBE	SMD	-623.49624	5.48(0)	3.02	64.21	-234.21
HSO ₃ ⁻	C ₁	PBE	SMD	-624.24488	12.29(0)	3.53	69.63	-63.78
H ₂ SO ₃	C _s	PBE	SMD	-624.77117	19.30(0)	3.82	71.77	-9.02
SO ₃ ²⁻	C _{3v}	BVP86	UFF	-623.95859	5.45(0)	3.03	64.24	-229.12
HSO ₃ ⁻	C ₁	BVP86	UFF	-624.70848	12.23(0)	3.54	69.72	-58.84
H ₂ SO ₃	C _s	BVP86	UFF	-625.23572	19.24(0)	3.83	71.84	-3.72
SO ₃ ²⁻	C _{3v}	BVP86	UAKS	-623.95859	5.45(0)	3.03	64.24	-222.26
HSO ₃ ⁻	C ₁	BVP86	UAKS	-624.70848	12.25(0)	3.53	69.62	-55.54
H ₂ SO ₃	C _s	BVP86	UAKS	-625.23572	19.24(0)	3.83	71.84	-3.24
SO ₃ ²⁻	C _{3v}	BVP86	Pauling	-623.95859	5.45(0)	3.03	64.24	-243.53
HSO ₃ ⁻	C ₁	BVP86	Pauling	-624.70848	12.23(0)	3.55	69.76	-66.37
H ₂ SO ₃	C _s	BVP86	Pauling	-625.23572	19.24(0)	3.83	71.84	-11.71
SO ₃ ²⁻	C _{3v}	BVP86	Klmat	-623.95859	5.45(0)	3.03	64.24	-230.44
HSO ₃ ⁻	C ₁	BVP86	Klamt	-624.70848	12.23(0)	3.55	69.77	-59.82
H ₂ SO ₃	C _s	BVP86	Klmat	-625.23572	19.24(0)	3.83	71.84	-5.52
SO ₃ ²⁻	C _{3v}	BVP86	SMD	-623.95859	5.45(0)	3.03	64.24	-235.37
HSO ₃ ⁻	C ₁	BVP86	SMD	-624.70848	12.23(0)	3.55	69.77	-63.22
H ₂ SO ₃	C _s	BVP86	SMD	-625.23572	19.24(0)	3.83	71.84	-9.10
SO ₃ ²⁻	C _{3v}	M052X	UFF	-623.84443	6.17(0)	2.89	63.43	-235.74
HSO ₃ ⁻	C ₁	M052X	UFF	-624.59720	13.34(0)	3.34	68.34	-61.76
H ₂ SO ₃	C _s	M052X	UFF	-625.12652	20.61(0)	3.63	70.27	-4.99
SO ₃ ²⁻	C _{3v}	M052X	UAKS	-623.84443	6.17(0)	2.89	63.43	-227.79
HSO ₃ ⁻	C ₁	M052X	UAKS	-624.59719	13.35(0)	3.33	68.28	-57.67
H ₂ SO ₃	C _s	M052X	UAKS	-625.12652	20.61(0)	3.63	70.27	-4.23
SO ₃ ²⁻	C _{3v}	M052X	Pauling	-623.84443	6.17(0)	2.89	63.43	-253.21
HSO ₃ ⁻	C ₁	M052X	Pauling	-624.59719	13.31(0)	3.35	68.46	-71.15
H ₂ SO ₃	C _s	M052X	Pauling	-625.12652	20.61(0)	3.63	70.27	-13.75
SO ₃ ²⁻	C _{3v}	M052X	Klamt	-623.84443	6.17(0)	2.89	63.43	-237.30
HSO ₃ ⁻	C ₁	M052X	Klamt	-624.59719	13.29(0)	3.37	68.65	-62.96
H ₂ SO ₃	C _s	M052X	Klamt	-625.12652	20.61(0)	3.63	70.27	-6.91
SO ₃ ²⁻	C _{3v}	M052X	SMD	-623.84443	6.17(0)	2.89	63.43	-242.98
HSO ₃ ⁻	C ₁	M052X	SMD	-624.59719	13.29(0)	3.37	68.65	-67.58
H ₂ SO ₃	C _s	M052X	SMD	-625.12652	20.61(0)	3.63	70.27	-10.55
SO ₄ ²⁻	T _d	B3LYP	UFF	-699.18733	9.25(0)	3.18	63.72	-225.59
HSO ₄ ⁻	C _s	B3LYP	UFF	-699.91122	16.52(0)	3.78	73.59	-59.49
H ₂ SO ₄	C ₂	B3LYP	UFF	-700.41831	24.17(0)	3.89	71.40	-5.93
SO ₄ ²⁻	T _d	B3LYP	UAKS	-699.18733	9.25(0)	3.18	63.72	-233.95
HSO ₄ ⁻	C _s	B3LYP	UAKS	-699.91122	16.52(0)	3.78	73.59	-66.76
H ₂ SO ₄	C ₂	B3LYP	UAKS	-700.41831	24.17(0)	3.89	71.40	-15.76
SO ₄ ²⁻	T _d	B3LYP	Pauling	-699.18733	9.25(0)	3.18	63.72	-241.52
HSO ₄ ⁻	C _s	B3LYP	Pauling	-699.91122	16.52(0)	3.78	73.59	-68.38
H ₂ SO ₄	C ₂	B3LYP	Pauling	-700.41831	24.17(0)	3.89	71.40	-16.09
SO ₄ ²⁻	T _d	B3LYP	Klamt	-699.18733	9.25(0)	3.18	63.72	-227.73
HSO ₄ ⁻	C _s	B3LYP	Klamt	-699.91122	16.52(0)	3.78	73.59	-61.28
H ₂ SO ₄	C ₂	B3LYP	Klamt	-700.41832	24.17(0)	3.89	71.41	-8.93

SO ₄ ²⁻	T _d	B3LYP	SMD	-699.18733	9.25 (0)	3.18	63.72	-234.08
HSO ₄ ⁻	C _s	B3LYP	SMD	-699.91122	16.52 (0)	3.78	73.59	-65.92
H ₂ SO ₄	C ₂	B3LYP	SMD	-700.41832	24.17 (0)	3.89	71.41	-12.76
SO ₄ ²⁻	T _d	PBE	UFF	-698.71636	8.80 (0)	3.27	64.23	-223.72
HSO ₄ ⁻	C ₁	PBE	UFF	-699.43954	15.76 (0)	3.95	77.85	-58.03
H ₂ SO ₄	C ₁	PBE	UFF	-699.94622	23.28 (0)	4.00	72.06	-5.11
SO ₄ ²⁻	T _d	PBE	UAKS	-698.71636	8.80 (0)	3.27	64.23	-231.80
HSO ₄ ⁻	C ₁	PBE	UAKS	-699.43954	15.76 (0)	3.95	77.85	-65.44
H ₂ SO ₄	C ₁	PBE	UAKS	-699.94622	23.28 (0)	4.00	72.06	-14.78
SO ₄ ²⁻	T _d	PBE	Pauling	-698.71636	8.80 (0)	3.27	64.23	-238.49
HSO ₄ ⁻	C ₁	PBE	Pauling	-699.43954	15.76 (0)	3.95	77.85	-66.61
H ₂ SO ₄	C ₁	PBE	Pauling	-699.94622	23.28 (0)	4.00	72.06	-14.94
SO ₄ ²⁻	T _d	PBE	Klamt	-698.71636	8.79 (0)	3.27	64.24	-225.75
HSO ₄ ⁻	C ₁	PBE	Klamt	-699.43954	15.76 (0)	3.95	77.78	-59.74
H ₂ SO ₄	C ₁	PBE	Klamt	-699.94622	23.28 (0)	4.00	72.06	-8.01
SO ₄ ²⁻	T _d	PBE	SMD	-698.71636	8.79 (0)	3.27	64.24	-231.56
HSO ₄ ⁻	C ₁	PBE	SMD	-699.43954	15.76 (0)	3.95	77.78	-64.31
H ₂ SO ₄	C ₁	PBE	SMD	-699.94622	23.28 (0)	4.00	72.06	-11.63
SO ₄ ²⁻	T _d	BVP86	UFF	-699.25677	8.77 (0)	3.27	64.25	-224.50
HSO ₄ ⁻	C ₁	BVP86	UFF	-699.98084	15.72 (0)	3.95	77.40	-58.30
H ₂ SO ₄	C ₁	BVP86	UFF	-700.48822	23.23 (0)	4.00	72.09	-5.15
SO ₄ ²⁻	T _d	BVP86	UAKS	-699.25677	8.77 (0)	3.27	64.25	-232.67
HSO ₄ ⁻	C ₁	BVP86	UAKS	-699.98084	15.72 (0)	3.95	77.40	-65.69
H ₂ SO ₄	C ₁	BVP86	UAKS	-700.48822	23.23 (0)	4.00	72.09	-14.81
SO ₄ ²⁻	T _d	BVP86	Pauling	-699.25677	8.77 (0)	3.27	64.25	-239.65
HSO ₄ ⁻	C ₁	BVP86	Pauling	-699.98084	15.72 (0)	3.95	77.40	-67.11
H ₂ SO ₄	C ₁	BVP86	Pauling	-700.48822	23.23 (0)	4.00	72.09	-15.06
SO ₄ ²⁻	T _d	BVP86	Klamt	-699.25677	8.76 (0)	3.27	64.25	-226.55
HSO ₄ ⁻	C ₁	BVP86	Klamt	-699.98084	15.72 (0)	3.95	77.39	-60.07
H ₂ SO ₄	C ₁	BVP86	Klamt	-700.48822	23.23 (0)	4.00	72.09	-8.05
SO ₄ ²⁻	T _d	BVP86	SMD	-699.25677	8.76 (0)	3.27	64.25	-232.51
HSO ₄ ⁻	C ₁	BVP86	SMD	-699.98084	15.72 (0)	3.95	77.39	-64.66
H ₂ SO ₄	C ₁	BVP86	SMD	-700.48822	23.23 (0)	4.00	72.09	-11.70
SO ₄ ²⁻	T _d	M052X	UFF	-699.14473	9.74 (0)	3.11	63.33	-228.41
HSO ₄ ⁻	C _s	M052X	UFF	-699.86492	17.06 (0)	3.71	73.59	-61.04
H ₂ SO ₄	C ₂	M052X	UFF	-700.36830	24.71 (0)	3.83	71.02	-6.91
SO ₄ ²⁻	T _d	M052X	UAKS	-699.14473	9.74 (0)	3.11	63.33	-237.07
HSO ₄ ⁻	C _s	M052X	UAKS	-699.86492	17.07 (0)	3.70	73.25	-68.51
H ₂ SO ₄	C ₂	M052X	UAKS	-700.36830	24.71 (0)	3.83	71.02	-16.92
SO ₄ ²⁻	T _d	M052X	Pauling	-699.14473	9.74 (0)	3.11	63.33	-245.88
HSO ₄ ⁻	C _s	M052X	Pauling	-699.86492	17.07 (0)	3.70	73.25	-70.95
H ₂ SO ₄	C ₂	M052X	Pauling	-700.36830	24.71 (0)	3.83	71.02	-17.70
SO ₄ ²⁻	T _d	M052X	Klamt	-699.14473	9.74 (0)	3.11	63.33	-230.67
HSO ₄ ⁻	C _s	M052X	Klamt	-699.86492	17.07 (0)	3.70	73.25	-62.95
H ₂ SO ₄	C ₂	M052X	Klamt	-700.36830	24.70 (0)	3.83	71.02	-10.00
SO ₄ ²⁻	T _d	M052X	SMD	-699.14473	9.74 (0)	3.11	63.33	-237.17
HSO ₄ ⁻	C _s	M052X	SMD	-699.86492	17.07 (0)	3.70	73.25	-67.63

H ₂ SO ₄	C ₂	M052X	SMD	-700.36830	24.70(0)	3.83	71.02	-13.80
C ₂ O ₄ ²⁻	D _{2d}	B3LYP	UFF	-377.24423	14.40(0)	3.81	71.46	-213.35
HC ₂ O ₄ ⁻	C _s	B3LYP	UFF	-377.95099	22.14(0)	4.07	76.16	-58.86
H ₂ C ₂ O ₄	C _{2h}	B3LYP	UFF	-378.48315	30.58(0)	4.11	76.95	-5.58
C ₂ O ₄ ²⁻	D _{2d}	B3LYP	UAKS	-377.24423	14.40(0)	3.81	71.46	-222.80
HC ₂ O ₄ ⁻	C _s	B3LYP	UAKS	-377.95099	22.14(0)	4.07	76.16	-66.67
H ₂ C ₂ O ₄	C _{2h}	B3LYP	UAKS	-378.48315	30.58(0)	4.11	76.95	-13.98
C ₂ O ₄ ²⁻	D _{2d}	B3LYP	Pauling	-377.24423	14.40(0)	3.81	71.46	-228.01
HC ₂ O ₄ ⁻	C _s	B3LYP	Pauling	-377.95099	22.14(0)	4.07	76.16	-69.93
H ₂ C ₂ O ₄	C _{2h}	B3LYP	Pauling	-378.48315	30.58(0)	4.11	76.95	-19.35
C ₂ O ₄ ²⁻	D _{2d}	B3LYP	Klamt	-377.24423	14.40(0)	3.81	71.46	-214.92
HC ₂ O ₄ ⁻	C _s	B3LYP	Klamt	-377.95099	22.14(0)	4.07	76.16	-60.52
H ₂ C ₂ O ₄	C _{2h}	B3LYP	Klamt	-378.48315	30.58(0)	4.11	76.95	-7.51
C ₂ O ₄ ²⁻	D _{2d}	B3LYP	SMD	-377.24423	14.40(0)	3.81	71.46	-221.86
HC ₂ O ₄ ⁻	C _s	B3LYP	SMD	-377.95099	22.14(0)	4.07	76.16	-64.28
H ₂ C ₂ O ₄	C _{2h}	B3LYP	SMD	-378.48315	30.58(0)	4.11	76.95	-11.00
C ₂ O ₄ ²⁻	D _{2d}	PBE	UFF	-376.86088	13.77(0)	3.88	71.92	-211.00
HC ₂ O ₄ ⁻	C _s	PBE	UFF	-377.56577	21.26(0)	4.14	76.57	-57.59
H ₂ C ₂ O ₄	C _{2h}	PBE	UFF	-378.09449	29.57(0)	4.18	77.43	-4.73
C ₂ O ₄ ²⁻	D _{2d}	PBE	UAKS	-376.86088	13.77(0)	3.88	71.92	-219.99
HC ₂ O ₄ ⁻	C _s	PBE	UAKS	-377.56577	21.26(0)	4.14	76.57	-65.12
H ₂ C ₂ O ₄	C _{2h}	PBE	UAKS	-378.09449	29.57(0)	4.18	77.37	-13.79
C ₂ O ₄ ²⁻	D _{2d}	PBE	Pauling	-376.86088	13.77(0)	3.88	71.92	-224.24
HC ₂ O ₄ ⁻	C _s	PBE	Pauling	-377.56577	21.26(0)	4.14	76.57	-67.02
H ₂ C ₂ O ₄	C _{2h}	PBE	Pauling	-378.09449	29.57(0)	4.18	77.43	-17.15
C ₂ O ₄ ²⁻	D _{2d}	PBE	Klamt	-376.86088	13.77(0)	3.88	71.92	-212.45
HC ₂ O ₄ ⁻	C _s	PBE	Klamt	-377.56577	21.26(0)	4.14	76.56	-59.21
H ₂ C ₂ O ₄	C _{2h}	PBE	Klamt	-378.09449	29.57(0)	4.18	77.44	-7.11
C ₂ O ₄ ²⁻	D _{2d}	PBE	SMD	-376.86088	13.77(0)	3.88	71.92	-218.99
HC ₂ O ₄ ⁻	C _s	PBE	SMD	-377.56577	21.26(0)	4.14	76.56	-62.41
H ₂ C ₂ O ₄	C _{2h}	PBE	SMD	-378.09449	29.57(0)	4.18	77.44	-10.03
C ₂ O ₄ ²⁻	D _{2d}	BVP86	UFF	-377.28170	13.74(0)	3.88	71.87	-211.94
HC ₂ O ₄ ⁻	C _s	BVP86	UFF	-377.98765	21.21(0)	4.14	76.56	-57.92
H ₂ C ₂ O ₄	C _{2h}	BVP86	UFF	-378.51710	29.49(0)	4.19	78.50	-4.79
C ₂ O ₄ ²⁻	D _{2d}	BVP86	UAKS	-377.28170	13.74(0)	3.88	71.87	-221.08
HC ₂ O ₄ ⁻	C _s	BVP86	UAKS	-377.98765	21.21(0)	4.14	76.56	-65.48
H ₂ C ₂ O ₄	C _{2h}	BVP86	UAKS	-378.51710	29.49(0)	4.19	78.50	-13.82
C ₂ O ₄ ²⁻	D _{2d}	BVP86	Pauling	-377.28170	13.74(0)	3.88	71.87	-225.61
HC ₂ O ₄ ⁻	C _s	BVP86	Pauling	-377.98765	21.21(0)	4.14	76.56	-67.60
H ₂ C ₂ O ₄	C _{2h}	BVP86	Pauling	-378.51710	29.49(0)	4.19	78.50	-17.34
C ₂ O ₄ ²⁻	D _{2d}	BVP86	Klamt	-377.28170	13.74(0)	3.88	71.88	-213.43
HC ₂ O ₄ ⁻	C _s	BVP86	Klamt	-377.98765	21.21(0)	4.14	76.56	-59.37
H ₂ C ₂ O ₄	C _{2h}	BVP86	Klamt	-378.51710	29.49(0)	4.19	78.50	-7.18
C ₂ O ₄ ²⁻	D _{2d}	BVP86	SMD	-377.28170	13.74(0)	3.88	71.88	-220.20
HC ₂ O ₄ ⁻	C _s	BVP86	SMD	-377.98765	21.21(0)	4.14	76.56	-62.83
H ₂ C ₂ O ₄	C _{2h}	BVP86	SMD	-378.51710	29.49(0)	4.19	78.50	-10.26

$C_2O_4^{2-}$	D_{2d}	M052X	UFF	-377.20607	14.97(0)	3.78	71.35	-216.45
$HC_2O_4^-$	C_s	M052X	UFF	-377.91051	22.78(0)	4.05	76.38	-60.57
$H_2C_2O_4$	C_{2h}	M052X	UFF	-378.44201	31.24(0)	4.06	75.55	-6.04
$C_2O_4^{2-}$	D_{2d}	M052X	UAKS	-377.20607	14.97(0)	3.78	71.35	-226.33
$HC_2O_4^-$	C_s	M052X	UAKS	-377.91051	22.78(0)	4.05	76.38	-68.60
$H_2C_2O_4$	C_{2h}	M052X	UAKS	-378.44201	31.24(0)	4.06	75.55	-14.99
$C_2O_4^{2-}$	D_{2d}	M052X	Pauling	-377.20607	14.97(0)	3.78	71.35	-232.72
$HC_2O_4^-$	C_s	M052X	Pauling	-377.91051	22.78(0)	4.05	76.38	-72.34
$H_2C_2O_4$	C_{2h}	M052X	Pauling	-378.44201	31.24(0)	4.06	75.55	-20.54
$C_2O_4^{2-}$	D_{2d}	M052X	Klamt	-377.20607	14.97(0)	3.78	71.35	-218.09
$HC_2O_4^-$	C_s	M052X	Klamt	-377.91051	22.78(0)	4.05	76.38	-62.34
$H_2C_2O_4$	C_{2h}	M052X	Klamt	-378.44201	31.24(0)	4.06	75.55	-8.49
$C_2O_4^{2-}$	D_{2d}	M052X	SMD	-377.20607	14.97(0)	3.78	71.35	-225.79
$HC_2O_4^-$	C_s	M052X	SMD	-377.91051	22.78(0)	4.05	76.38	-66.25
$H_2C_2O_4$	C_{2h}	M052X	SMD	-378.44201	31.24(0)	4.06	75.55	-11.99
$C_3H_2O_4^{2-}$	C_s	B3LYP	UFF	-416.58947	31.72(0)	4.70	85.68	-200.81
$HC_3H_2O_4^-$	C_1	B3LYP	UFF	-417.30938	39.14(0)	4.52	81.77	-51.76
$H_2C_3H_2O_4$	C_1	B3LYP	UFF	-417.82894	48.53(0)	4.79	84.09	-6.01
$C_3H_2O_4^{2-}$	C_s	B3LYP	UAKS	-416.58947	31.72(0)	4.70	85.68	-212.69
$HC_3H_2O_4^-$	C_1	B3LYP	UAKS	-417.30938	39.14(0)	4.52	81.77	-57.38
$H_2C_3H_2O_4$	C_1	B3LYP	UAKS	-417.82894	48.53(0)	4.79	84.09	-14.34
$C_3H_2O_4^{2-}$	C_s	B3LYP	Pauling	-416.58947	31.72(0)	4.70	85.68	-217.24
$HC_3H_2O_4^-$	C_1	B3LYP	Pauling	-417.30938	39.14(0)	4.52	81.77	-63.02
$H_2C_3H_2O_4$	C_1	B3LYP	Pauling	-417.82894	48.53(0)	4.79	84.09	-19.40
$C_3H_2O_4^{2-}$	C_s	B3LYP	Klamt	-416.58947	31.72(0)	4.70	85.68	-202.87
$HC_3H_2O_4^-$	C_1	B3LYP	Klamt	-417.30938	39.14(0)	4.52	81.77	-53.73
$H_2C_3H_2O_4$	C_1	B3LYP	Klamt	-417.82894	48.52(0)	4.79	84.09	-8.68
$C_3H_2O_4^{2-}$	C_s	B3LYP	SMD	-416.58947	31.72(0)	4.70	85.68	-211.68
$HC_3H_2O_4^-$	C_1	B3LYP	SMD	-417.30938	39.14(0)	4.52	81.77	-56.74
$H_2C_3H_2O_4$	C_1	B3LYP	SMD	-417.82894	48.52(0)	4.79	84.09	-12.36
$C_3H_2O_4^{2-}$	C_s	PBE	UFF	-416.14727	30.59(0)	4.77	84.77	-198.33
$HC_3H_2O_4^-$	C_1	PBE	UFF	-416.86818	37.11(0)	4.64	82.21	-50.61
$H_2C_3H_2O_4$	C_1	PBE	UFF	-417.38260	47.00(0)	4.82	83.18	-5.09
$C_3H_2O_4^{2-}$	C_s	PBE	UAKS	-416.14727	30.59(0)	4.77	84.77	-209.80
$HC_3H_2O_4^-$	C_1	PBE	UAKS	-416.86818	37.11(0)	4.64	82.21	-56.20
$H_2C_3H_2O_4$	C_1	PBE	UAKS	-417.38260	47.00(0)	4.82	83.18	-14.29
$C_3H_2O_4^{2-}$	C_s	PBE	Pauling	-416.14727	30.59(0)	4.77	84.77	-213.25
$HC_3H_2O_4^-$	C_1	PBE	Pauling	-416.86818	37.11(0)	4.64	82.21	-59.88
$H_2C_3H_2O_4$	C_1	PBE	Pauling	-417.38260	47.00(0)	4.82	83.18	-17.05
$C_3H_2O_4^{2-}$	C_s	PBE	Klamt	-416.14727	30.59(0)	4.77	84.77	-200.30
$HC_3H_2O_4^-$	C_1	PBE	Klamt	-416.86818	37.11(0)	4.64	82.21	-52.27
$H_2C_3H_2O_4$	C_1	PBE	Klamt	-417.38259	46.99(0)	4.82	83.20	-7.73
$C_3H_2O_4^{2-}$	C_s	PBE	SMD	-416.14727	30.59(0)	4.77	84.77	-208.63
$HC_3H_2O_4^-$	C_1	PBE	SMD	-416.86818	37.11(0)	4.64	82.21	-54.76
$H_2C_3H_2O_4$	C_1	PBE	SMD	-417.38259	46.99(0)	4.82	83.20	-11.22
$C_3H_2O_4^{2-}$	C_s	BVP86	UFF	-416.62523	30.54(0)	4.78	85.11	-199.18
$HC_3H_2O_4^-$	C_1	BVP86	UFF	-417.34714	37.03(0)	4.66	82.27	-50.92

H ₂ C ₃ H ₂ O ₄	C ₁	BVP86	UFF	-417.86235	46.94 (0)	4.82	83.28	-5.17
C ₃ H ₂ O ₄ ²⁻	C _s	BVP86	UAKS	-416.62523	30.54 (0)	4.78	85.11	-210.80
HC ₃ H ₂ O ₄ ⁻	C ₁	BVP86	UAKS	-417.34714	37.03 (0)	4.66	82.27	-56.45
H ₂ C ₃ H ₂ O ₄	C ₁	BVP86	UAKS	-417.86235	46.94 (0)	4.82	83.28	-14.30
C ₃ H ₂ O ₄ ²⁻	C _s	BVP86	Pauling	-416.62523	30.54 (0)	4.78	85.11	-214.53
HC ₃ H ₂ O ₄ ⁻	C ₁	BVP86	Pauling	-417.34714	37.03 (0)	4.66	82.27	-60.48
H ₂ C ₃ H ₂ O ₄	C ₁	BVP86	Pauling	-417.86235	46.94 (0)	4.82	83.28	-17.27
C ₃ H ₂ O ₄ ²⁻	C _s	BVP86	Klamt	-416.62523	30.54 (0)	4.78	85.04	-201.18
HC ₃ H ₂ O ₄ ⁻	C ₁	BVP86	Klamt	-417.34714	37.03 (0)	4.66	82.27	-52.60
H ₂ C ₃ H ₂ O ₄	C ₁	BVP86	Klamt	-417.86235	46.94 (0)	4.82	83.30	-7.82
C ₃ H ₂ O ₄ ²⁻	C _s	BVP86	SMD	-416.62523	30.54 (0)	4.78	85.04	-209.72
HC ₃ H ₂ O ₄ ⁻	C ₁	BVP86	SMD	-417.34714	37.03 (0)	4.66	82.27	-55.24
H ₂ C ₃ H ₂ O ₄	C ₁	BVP86	SMD	-417.86235	46.94 (0)	4.82	83.30	-11.35
C ₃ H ₂ O ₄ ²⁻	C _s	M052X	UFF	-416.54713	32.67 (0)	4.63	84.23	-204.43
HC ₃ H ₂ O ₄ ⁻	C ₁	M052X	UFF	-417.26899	39.91 (0)	4.41	80.71	-53.05
H ₂ C ₃ H ₂ O ₄	C ₁	M052X	UFF	-417.78425	49.41 (0)	4.77	84.68	-6.40
C ₃ H ₂ O ₄ ²⁻	C _s	M052X	UAKS	-416.54713	32.67 (0)	4.63	84.23	-216.97
HC ₃ H ₂ O ₄ ⁻	C ₁	M052X	UAKS	-417.26899	39.91 (0)	4.41	80.71	-58.63
H ₂ C ₃ H ₂ O ₄	C ₁	M052X	UAKS	-417.78425	49.41 (0)	4.77	84.68	-15.49
C ₃ H ₂ O ₄ ²⁻	C _s	M052X	Pauling	-416.54713	32.67 (0)	4.63	84.23	-222.75
HC ₃ H ₂ O ₄ ⁻	C ₁	M052X	Pauling	-417.26899	39.91 (0)	4.41	80.71	-64.33
H ₂ C ₃ H ₂ O ₄	C ₁	M052X	Pauling	-417.78425	49.41 (0)	4.77	84.68	-20.47
C ₃ H ₂ O ₄ ²⁻	C _s	M052X	Klamt	-416.54713	32.67 (0)	4.63	84.23	-206.64
HC ₃ H ₂ O ₄ ⁻	C ₁	M052X	Klamt	-417.26899	39.91 (0)	4.41	80.71	-54.94
H ₂ C ₃ H ₂ O ₄	C ₁	M052X	Klamt	-417.78426	49.39 (0)	4.77	84.28	-9.14
C ₃ H ₂ O ₄ ²⁻	C _s	M052X	SMD	-416.54713	32.67 (0)	4.63	84.23	-216.43
HC ₃ H ₂ O ₄ ⁻	C ₁	M052X	SMD	-417.26899	39.91 (0)	4.41	80.71	-58.24
H ₂ C ₃ H ₂ O ₄	C ₁	M052X	SMD	-417.78426	49.39 (0)	4.77	84.28	-13.21
HPO ₃ ²⁻	C _{3v}	B3LYP	UFF	-567.76830	11.76 (0)	2.97	64.05	-229.09
H ₂ PO ₃ ⁻	C ₁	B3LYP	UFF	-568.51148	19.69 (0)	3.33	68.34	-62.26
H ₃ PO ₃	C ₁	B3LYP	UFF	-569.04709	26.88 (0)	3.86	72.13	-6.97
HPO ₃ ²⁻	C _{3v}	B3LYP	UAKS	-567.76830	11.76 (0)	2.97	64.05	-229.25
H ₂ PO ₃ ⁻	C ₁	B3LYP	UAKS	-568.51148	19.69 (0)	3.33	68.34	-63.34
H ₃ PO ₃	C ₁	B3LYP	UAKS	-569.04710	26.87 (0)	3.87	72.24	-9.63
HPO ₃ ²⁻	C _{3v}	B3LYP	Pauling	-567.76830	11.76 (0)	2.97	64.05	-246.09
H ₂ PO ₃ ⁻	C ₁	B3LYP	Pauling	-568.51148	19.69 (0)	3.33	68.34	-72.91
H ₃ PO ₃	C ₁	B3LYP	Pauling	-569.04709	26.88 (0)	3.86	72.13	-17.87
HPO ₃ ²⁻	C _{3v}	B3LYP	Klamt	-567.76830	11.76 (0)	2.97	64.05	-230.67
H ₂ PO ₃ ⁻	C ₁	B3LYP	Klamt	-568.51148	19.69 (0)	3.33	68.34	-63.90
H ₃ PO ₃	C ₁	B3LYP	Klamt	-569.04709	26.88 (0)	3.86	72.13	-9.37
HPO ₃ ²⁻	C _{3v}	B3LYP	SMD	-567.76830	11.76 (0)	2.97	64.05	-237.27
H ₂ PO ₃ ⁻	C ₁	B3LYP	SMD	-568.51148	19.69 (0)	3.33	68.34	-66.37
H ₃ PO ₃	C ₁	B3LYP	SMD	-569.04709	26.88 (0)	3.86	72.13	-11.36
HPO ₃ ²⁻	C _{3v}	PBE	UFF	-567.36540	11.08 (0)	3.05	64.51	-225.81
H ₂ PO ₃ ⁻	C ₁	PBE	UFF	-568.10375	18.87 (0)	3.41	68.80	-60.66
H ₃ PO ₃	C ₁	PBE	UFF	-568.63581	25.95 (0)	3.92	72.51	-5.94
HPO ₃ ²⁻	C _{3v}	PBE	UAKS	-567.36540	11.08 (0)	3.05	64.51	-226.02

H ₂ PO ₃ ⁻	C ₁	PBE	UAKS	-568.10375	18.87(0)	3.41	68.80	-62.02
H ₃ PO ₃	C ₁	PBE	UAKS	-568.63580	25.95(0)	3.92	72.56	-9.30
HPO ₃ ²⁻	C _{3v}	PBE	Pauling	-567.36540	11.08(0)	3.05	64.51	-241.07
H ₂ PO ₃ ⁻	C ₁	PBE	Pauling	-568.10375	18.87(0)	3.41	68.80	-70.17
H ₃ PO ₃	C ₁	PBE	Pauling	-568.63581	25.95(0)	3.92	72.51	-16.12
HPO ₃ ²⁻	C _{3v}	PBE	Klamt	-567.36540	11.08(0)	3.05	64.51	-227.25
H ₂ PO ₃ ⁻	C ₁	PBE	Klamt	-568.10375	18.87(0)	3.41	68.80	-62.20
H ₃ PO ₃	C ₁	PBE	Klamt	-568.63581	25.95(0)	3.92	72.51	-8.75
HPO ₃ ²⁻	C _{3v}	PBE	SMD	-567.36540	11.08(0)	3.05	64.51	-233.02
H ₂ PO ₃ ⁻	C ₁	PBE	SMD	-568.10375	18.87(0)	3.41	68.80	-64.21
H ₃ PO ₃	C ₁	PBE	SMD	-568.63581	25.95(0)	3.92	72.51	-10.03
HPO ₃ ²⁻	C _{3v}	BVP86	UFF	-567.81452	11.10(0)	3.05	64.48	-226.85
H ₂ PO ₃ ⁻	C ₁	BVP86	UFF	-568.55388	18.87(0)	3.40	68.79	-61.05
H ₃ PO ₃	C ₁	BVP86	UFF	-569.08690	25.97(0)	3.91	72.35	-6.05
HPO ₃ ²⁻	C _{3v}	BVP86	UAKS	-567.81452	11.10(0)	3.05	64.48	-227.02
H ₂ PO ₃ ⁻	C ₁	BVP86	UAKS	-568.55388	18.87(0)	3.40	68.78	-62.32
H ₃ PO ₃	C ₁	BVP86	UAKS	-569.08690	25.95(0)	3.92	72.49	-9.35
HPO ₃ ²⁻	C _{3v}	BVP86	Pauling	-567.81452	11.10(0)	3.05	64.48	-242.53
H ₂ PO ₃ ⁻	C ₁	BVP86	Pauling	-568.55388	18.87(0)	3.40	68.78	-70.84
H ₃ PO ₃	C ₁	BVP86	Pauling	-569.08690	25.97(0)	3.91	72.35	-16.34
HPO ₃ ²⁻	C _{3v}	BVP86	Klamt	-567.81452	11.10(0)	3.05	64.48	-228.33
H ₂ PO ₃ ⁻	C ₁	BVP86	Klamt	-568.55388	18.87(0)	3.40	68.79	-62.61
H ₃ PO ₃	C ₁	BVP86	Klamt	-569.08690	25.97(0)	3.91	72.35	-8.86
HPO ₃ ²⁻	C _{3v}	BVP86	SMD	-567.81452	11.10(0)	3.05	64.48	-234.28
H ₂ PO ₃ ⁻	C ₁	BVP86	SMD	-568.55388	18.87(0)	3.40	68.79	-64.78
H ₃ PO ₃	C ₁	BVP86	SMD	-569.08690	25.97(0)	3.91	72.35	-10.19
HPO ₃ ²⁻	C _{3v}	M052X	UFF	-567.72507	12.25(0)	2.92	63.78	-233.34
H ₂ PO ₃ ⁻	C ₁	M052X	UFF	-568.46950	20.24(0)	3.27	67.97	-64.22
H ₃ PO ₃	C ₁	M052X	UFF	-569.00509	27.35(0)	3.85	72.31	-7.55
HPO ₃ ²⁻	C _{3v}	M052X	UAKS	-567.72507	12.25(0)	2.92	63.78	-233.19
H ₂ PO ₃ ⁻	C ₁	M052X	UAKS	-568.46951	20.27(0)	3.27	67.98	-64.98
H ₃ PO ₃	C ₁	M052X	UAKS	-569.00509	27.40(0)	3.80	71.72	-10.34
HPO ₃ ²⁻	C _{3v}	M052X	Pauling	-567.72507	12.25(0)	2.92	63.78	-252.39
H ₂ PO ₃ ⁻	C ₁	M052X	Pauling	-568.46951	20.27(0)	3.27	67.98	-76.18
H ₃ PO ₃	C ₁	M052X	Pauling	-569.00509	27.35(0)	3.85	72.31	-19.21
HPO ₃ ²⁻	C _{3v}	M052X	Klamt	-567.72507	12.25(0)	2.92	63.78	-235.05
H ₂ PO ₃ ⁻	C ₁	M052X	Klamt	-568.46950	20.24(0)	3.27	67.97	-65.99
H ₃ PO ₃	C ₁	M052X	Klamt	-569.00509	27.35(0)	3.85	72.31	-10.49
HPO ₃ ²⁻	C _{3v}	M052X	SMD	-567.72507	12.25(0)	2.92	63.78	-242.65
H ₂ PO ₃ ⁻	C ₁	M052X	SMD	-568.46950	20.24(0)	3.27	67.97	-69.05
H ₃ PO ₃	C ₁	M052X	SMD	-569.00509	27.35(0)	3.85	72.31	-12.49
C ₂ H ₂ O ₂ S ²⁻	C _s	B3LYP	UFF	-626.14461	24.49(0)	3.78	75.05	-205.74
HC ₂ H ₂ O ₂ S ⁻	C _s	B3LYP	UFF	-626.85928	30.23(0)	3.96	75.09	-55.55
H ₂ C ₂ H ₂ O ₂ S	C _s	B3LYP	UFF	-627.40046	38.47(0)	4.30	77.84	-3.15
C ₂ H ₂ O ₂ S ²⁻	C _s	B3LYP	UAKS	-626.14461	24.49(0)	3.78	75.05	-213.93
HC ₂ H ₂ O ₂ S ⁻	C _s	B3LYP	UAKS	-626.85928	30.23(0)	3.96	75.09	-60.97
H ₂ C ₂ H ₂ O ₂ S	C _s	B3LYP	UAKS	-627.40046	38.47(0)	4.30	77.84	-9.47

C ₂ H ₂ O ₂ S ²⁻	C _s	B3LYP	Pauling	-626.14461	24.49(0)	3.78	75.05	-215.98
HC ₂ H ₂ O ₂ S ⁻	C _s	B3LYP	Pauling	-626.85928	30.23(0)	3.96	75.09	-63.85
H ₂ C ₂ H ₂ O ₂ S	C _s	B3LYP	Pauling	-627.40046	38.47(0)	4.30	77.84	-12.17
C ₂ H ₂ O ₂ S ²⁻	C _s	B3LYP	Klamt	-626.14461	24.49(0)	3.78	75.05	-204.30
HC ₂ H ₂ O ₂ S ⁻	C _s	B3LYP	Klamt	-626.85928	30.23(0)	3.96	75.09	-56.25
H ₂ C ₂ H ₂ O ₂ S	C _s	B3LYP	Klamt	-627.40046	38.47(0)	4.30	77.84	-5.34
C ₂ H ₂ O ₂ S ²⁻	C _s	B3LYP	SMD	-626.14461	24.49(0)	3.78	75.05	-205.52
HC ₂ H ₂ O ₂ S ⁻	C _s	B3LYP	SMD	-626.85928	30.23(0)	3.96	75.09	-59.95
H ₂ C ₂ H ₂ O ₂ S	C _s	B3LYP	SMD	-627.40046	38.47(0)	4.30	77.84	-7.89
C ₂ H ₂ O ₂ S ²⁻	C _s	PBE	UFF	-625.70638	23.62(0)	3.85	75.73	-203.75
HC ₂ H ₂ O ₂ S ⁻	C _s	PBE	UFF	-626.41382	29.15(0)	4.18	76.67	-58.00
H ₂ C ₂ H ₂ O ₂ S	C _s	PBE	UFF	-626.95678	37.32(0)	4.35	78.08	-1.70
C ₂ H ₂ O ₂ S ²⁻	C _s	PBE	UAKS	-625.70638	23.62(0)	3.85	75.73	-211.80
HC ₂ H ₂ O ₂ S ⁻	C _s	PBE	UAKS	-626.41382	29.15(0)	4.18	76.67	-63.72
H ₂ C ₂ H ₂ O ₂ S	C _s	PBE	UAKS	-626.95678	37.32(0)	4.35	78.08	-9.73
C ₂ H ₂ O ₂ S ²⁻	C _s	PBE	Pauling	-625.70638	23.62(0)	3.85	75.73	-213.27
HC ₂ H ₂ O ₂ S ⁻	C _s	PBE	Pauling	-626.41382	29.15(0)	4.18	76.67	-66.18
H ₂ C ₂ H ₂ O ₂ S	C _s	PBE	Pauling	-626.95678	37.32(0)	4.35	78.08	-11.09
C ₂ H ₂ O ₂ S ²⁻	C _s	PBE	Klamt	-625.70638	23.62(0)	3.85	75.73	-202.24
HC ₂ H ₂ O ₂ S ⁻	C _s	PBE	Klamt	-626.41382	29.15(0)	4.18	76.67	-59.18
H ₂ C ₂ H ₂ O ₂ S	C _s	PBE	Klamt	-626.95678	37.32(0)	4.35	78.08	-4.80
C ₂ H ₂ O ₂ S ²⁻	C _s	PBE	SMD	-625.70638	23.62(0)	3.85	75.73	-203.30
HC ₂ H ₂ O ₂ S ⁻	C _s	PBE	SMD	-626.41382	29.15(0)	4.18	76.67	-62.36
H ₂ C ₂ H ₂ O ₂ S	C _s	PBE	SMD	-626.95678	37.32(0)	4.35	78.08	-7.46
C ₂ H ₂ O ₂ S ²⁻	C _s	BVP86	UFF	-626.19650	23.59(0)	3.85	75.80	-204.39
HC ₂ H ₂ O ₂ S ⁻	C _s	BVP86	UFF	-626.90427	29.11(0)	4.18	76.69	-58.36
H ₂ C ₂ H ₂ O ₂ S	C _s	BVP86	UFF	-627.44808	37.27(0)	4.35	78.14	-1.73
C ₂ H ₂ O ₂ S ²⁻	C _s	BVP86	UAKS	-626.19650	23.59(0)	3.85	75.80	-212.50
HC ₂ H ₂ O ₂ S ⁻	C _s	BVP86	UAKS	-626.90427	29.11(0)	4.18	76.69	-64.09
H ₂ C ₂ H ₂ O ₂ S	C _s	BVP86	UAKS	-627.44808	37.27(0)	4.35	78.14	-9.70
C ₂ H ₂ O ₂ S ²⁻	C _s	BVP86	Pauling	-626.19650	23.59(0)	3.85	75.80	-214.11
HC ₂ H ₂ O ₂ S ⁻	C _s	BVP86	Pauling	-626.90427	29.11(0)	4.18	76.69	-66.74
H ₂ C ₂ H ₂ O ₂ S	C _s	BVP86	Pauling	-627.44808	37.27(0)	4.35	78.14	-11.18
C ₂ H ₂ O ₂ S ²⁻	C _s	BVP86	Klamt	-626.19650	23.59(0)	3.85	75.80	-202.89
HC ₂ H ₂ O ₂ S ⁻	C _s	BVP86	Klamt	-626.90427	29.11(0)	4.18	76.69	-59.53
H ₂ C ₂ H ₂ O ₂ S	C _s	BVP86	Klamt	-627.44808	37.27(0)	4.35	78.14	-4.82
C ₂ H ₂ O ₂ S ²⁻	C _s	BVP86	SMD	-626.19650	23.59(0)	3.85	75.80	-203.99
HC ₂ H ₂ O ₂ S ⁻	C _s	BVP86	SMD	-626.90427	29.11(0)	4.18	76.69	-62.81
H ₂ C ₂ H ₂ O ₂ S	C _s	BVP86	SMD	-627.44808	37.27(0)	4.35	78.14	-7.49
C ₂ H ₂ O ₂ S ²⁻	C _s	M052X	UFF	-626.09557	25.26(0)	3.72	74.63	-209.73
HC ₂ H ₂ O ₂ S ⁻	C _s	M052X	UFF	-626.80919	31.28(0)	3.86	74.57	-57.56
H ₂ C ₂ H ₂ O ₂ S	C ₁	M052X	UFF	-627.35164	39.34(0)	4.28	78.36	-2.64
C ₂ H ₂ O ₂ S ²⁻	C _s	M052X	UAKS	-626.09557	25.26(0)	3.72	74.63	-218.27
HC ₂ H ₂ O ₂ S ⁻	C _s	M052X	UAKS	-626.80919	31.28(0)	3.86	74.57	-62.93
H ₂ C ₂ H ₂ O ₂ S	C ₁	M052X	UAKS	-627.35164	39.34(0)	4.28	78.36	-9.10
C ₂ H ₂ O ₂ S ²⁻	C _s	M052X	Pauling	-626.09557	25.26(0)	3.72	74.63	-221.11
HC ₂ H ₂ O ₂ S ⁻	C _s	M052X	Pauling	-626.80919	31.28(0)	3.86	74.57	-66.32

H ₂ C ₂ H ₂ O ₂ S	C ₁	M052X	Pauling	-627.35164	39.34 (0)	4.28	78.36	-11.25
C ₂ H ₂ O ₂ S ²⁻	C _s	M052X	Klamt	-626.09557	25.26 (0)	3.72	74.63	-208.25
HC ₂ H ₂ O ₂ S ⁻	C _s	M052X	Klamt	-626.80919	31.28 (0)	3.86	74.57	-58.38
H ₂ C ₂ H ₂ O ₂ S	C ₁	M052X	Klamt	-627.35164	39.34 (0)	4.28	78.36	-4.50
C ₂ H ₂ O ₂ S ²⁻	C _s	M052X	SMD	-626.09557	25.26 (0)	3.72	74.63	-209.89
HC ₂ H ₂ O ₂ S ⁻	C _s	M052X	SMD	-626.80919	31.28 (0)	3.86	74.57	-62.14
H ₂ C ₂ H ₂ O ₂ S	C ₁	M052X	SMD	-627.35164	39.34 (0)	4.28	78.36	-8.57
^f C ₄ H ₂ O ₄ ²⁻	C ₁	B3LYP	UFF	-454.69350	34.84 (0)	5.22	89.23	-193.67
^f HC ₄ H ₂ O ₄ ⁻	C _s	B3LYP	UFF	-455.40920	42.50 (0)	4.88	83.71	-49.92
^f H ₂ C ₄ H ₂ O ₄	C _s	B3LYP	UFF	-455.92464	52.22 (0)	5.12	85.67	-5.21
^f C ₄ H ₂ O ₄ ²⁻	C ₁	B3LYP	UAKS	-454.69350	34.84 (0)	5.22	89.23	-204.54
^f HC ₄ H ₂ O ₄ ⁻	C _s	B3LYP	UAKS	-455.40920	42.50 (0)	4.88	83.71	-53.98
^f H ₂ C ₄ H ₂ O ₄	C _s	B3LYP	UAKS	-455.92464	52.22 (0)	5.12	85.67	-12.01
^f C ₄ H ₂ O ₄ ²⁻	C ₁	B3LYP	Pauling	-454.69350	34.84 (0)	5.22	89.23	-209.21
^f HC ₄ H ₂ O ₄ ⁻	C _s	B3LYP	Pauling	-455.40920	42.50 (0)	4.88	83.71	-60.55
^f H ₂ C ₄ H ₂ O ₄	C _s	B3LYP	Pauling	-455.92464	52.22 (0)	5.12	85.67	-18.96
^f C ₄ H ₂ O ₄ ²⁻	C ₁	B3LYP	Klamt	-454.69350	34.84 (0)	5.22	89.23	-195.72
^f HC ₄ H ₂ O ₄ ⁻	C _s	B3LYP	Klamt	-455.40920	42.50 (0)	4.88	83.71	-51.23
^f H ₂ C ₄ H ₂ O ₄	C _s	B3LYP	Klamt	-455.92464	52.22 (0)	5.12	85.67	-7.34
^f C ₄ H ₂ O ₄ ²⁻	C ₁	B3LYP	SMD	-454.69350	34.84 (0)	5.22	89.23	-204.31
^f HC ₄ H ₂ O ₄ ⁻	C _s	B3LYP	SMD	-455.40920	42.50 (0)	4.88	83.71	-54.30
^f H ₂ C ₄ H ₂ O ₄	C _s	B3LYP	SMD	-455.92464	52.22 (0)	5.12	85.67	-11.10
^f C ₄ H ₂ O ₄ ²⁻	C ₁	PBE	UFF	-454.20573	33.55 (0)	5.34	90.10	-191.26
^f HC ₄ H ₂ O ₄ ⁻	C _s	PBE	UFF	-454.92030	40.45 (0)	5.01	84.41	-48.50
^f H ₂ C ₄ H ₂ O ₄	C _s	PBE	UFF	-455.43110	50.46 (0)	5.22	86.46	-4.36
^f C ₄ H ₂ O ₄ ²⁻	C ₁	PBE	UAKS	-454.20573	33.55 (0)	5.34	90.10	-201.67
^f HC ₄ H ₂ O ₄ ⁻	C _s	PBE	UAKS	-454.92030	40.45 (0)	5.01	84.41	-52.73
^f H ₂ C ₄ H ₂ O ₄	C _s	PBE	UAKS	-455.43110	50.46 (0)	5.22	86.46	-11.67
^f C ₄ H ₂ O ₄ ²⁻	C ₁	PBE	Pauling	-454.20573	33.55 (0)	5.34	90.10	-205.18
^f HC ₄ H ₂ O ₄ ⁻	C _s	PBE	Pauling	-454.92030	40.45 (0)	5.01	84.41	-57.49
^f H ₂ C ₄ H ₂ O ₄	C _s	PBE	Pauling	-455.43110	50.46 (0)	5.22	86.46	-16.79
^f C ₄ H ₂ O ₄ ²⁻	C ₁	PBE	Klamt	-454.20573	33.55 (0)	5.34	90.10	-193.17
^f HC ₄ H ₂ O ₄ ⁻	C _s	PBE	Klamt	-454.92030	40.45 (0)	5.01	84.41	-49.81
^f H ₂ C ₄ H ₂ O ₄	C _s	PBE	Klamt	-455.43110	50.46 (0)	5.22	86.46	-6.54
^f C ₄ H ₂ O ₄ ²⁻	C ₁	PBE	SMD	-454.20573	33.55 (0)	5.34	90.10	-201.28
^f HC ₄ H ₂ O ₄ ⁻	C _s	PBE	SMD	-454.92030	40.45 (0)	5.01	84.41	-52.48
^f H ₂ C ₄ H ₂ O ₄	C _s	PBE	SMD	-455.43110	50.46 (0)	5.22	86.46	-10.22
^f C ₄ H ₂ O ₄ ²⁻	C ₁	BVP86	UFF	-454.73231	33.51 (0)	5.34	90.12	-191.95
^f HC ₄ H ₂ O ₄ ⁻	C _s	BVP86	UFF	-455.44797	40.36 (0)	5.02	84.40	-48.83
^f H ₂ C ₄ H ₂ O ₄	C _s	BVP86	UFF	-455.95959	50.39 (0)	5.22	86.40	-3.25
^f C ₄ H ₂ O ₄ ²⁻	C ₁	BVP86	UAKS	-454.73231	33.51 (0)	5.34	90.12	-202.48
^f HC ₄ H ₂ O ₄ ⁻	C _s	BVP86	UAKS	-455.44797	40.36 (0)	5.02	84.40	-53.01
^f H ₂ C ₄ H ₂ O ₄	C _s	BVP86	UAKS	-455.95959	50.39 (0)	5.22	86.40	-11.71
^f C ₄ H ₂ O ₄ ²⁻	C ₁	BVP86	Pauling	-454.73231	33.51 (0)	5.34	90.12	-206.32
^f HC ₄ H ₂ O ₄ ⁻	C _s	BVP86	Pauling	-455.44797	40.36 (0)	5.02	84.40	-58.16
^f H ₂ C ₄ H ₂ O ₄	C _s	BVP86	Pauling	-455.95959	50.39 (0)	5.22	86.40	-17.00
^f C ₄ H ₂ O ₄ ²⁻	C ₁	BVP86	Klamt	-454.73231	33.51 (0)	5.34	90.12	-193.88

${}^f\text{HC}_4\text{H}_2\text{O}_4^-$	C_s	BVP86	Klamt	-455.44797	40.36 (0)	5.02	84.40	-50.14
${}^f\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_s	BVP86	Klamt	-455.95959	50.39 (0)	5.22	86.40	-6.61
${}^f\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_1	BVP86	SMD	-454.73231	33.51 (0)	5.34	90.12	-202.23
${}^f\text{HC}_4\text{H}_2\text{O}_4^-$	C_s	BVP86	SMD	-455.44797	40.36 (0)	5.02	84.40	-52.97
${}^f\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_s	BVP86	SMD	-455.95959	50.39 (0)	5.22	86.40	-10.36
${}^f\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_1	M052X	UFF	-454.64572	35.86 (0)	5.17	88.47	-197.63
${}^f\text{HC}_4\text{H}_2\text{O}_4^-$	C_s	M052X	UFF	-455.36428	42.95 (0)	4.85	83.43	-51.63
${}^f\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_s	M052X	UFF	-455.87459	53.06 (0)	5.11	85.80	-5.80
${}^f\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_1	M052X	UAKS	-454.64572	35.86 (0)	5.17	88.47	-208.90
${}^f\text{HC}_4\text{H}_2\text{O}_4^-$	C_s	M052X	UAKS	-455.36428	42.95 (0)	4.85	83.43	-55.09
${}^f\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_s	M052X	UAKS	-455.87459	53.06 (0)	5.11	85.80	-12.81
${}^f\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_1	M052X	Pauling	-454.64572	35.86 (0)	5.17	88.47	-214.97
${}^f\text{HC}_4\text{H}_2\text{O}_4^-$	C_s	M052X	Pauling	-455.36428	42.95 (0)	4.85	83.43	-62.34
${}^f\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_s	M052X	Pauling	-455.87459	53.06 (0)	5.11	85.80	-19.99
${}^f\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_1	M052X	Klamt	-454.64572	35.86 (0)	5.17	88.47	-199.75
${}^f\text{HC}_4\text{H}_2\text{O}_4^-$	C_s	M052X	Klamt	-455.36428	42.95 (0)	4.85	83.43	-52.42
${}^f\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_s	M052X	Klamt	-455.87459	53.06 (0)	5.11	85.80	-7.99
${}^f\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_1	M052X	SMD	-454.64572	35.86 (0)	5.17	88.47	-209.36
${}^f\text{HC}_4\text{H}_2\text{O}_4^-$	C_s	M052X	SMD	-455.36428	42.95 (0)	4.85	83.43	-55.61
${}^f\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_s	M052X	SMD	-455.87459	53.06 (0)	5.11	85.80	-11.75
$\text{C}_4\text{H}_5\text{NO}_4^{2-}$	C_s	B3LYP	UFF	-511.31958	60.04 (0)	6.19	96.24	-177.96
$\text{HC}_4\text{H}_5\text{NO}_4^-$	C_1	B3LYP	UFF	-511.99740	67.95 (0)	5.99	93.33	-50.09
$\text{H}_2\text{C}_4\text{H}_5\text{NO}_4$	C_s	B3LYP	UFF	-512.51258	77.46 (0)	6.36	96.68	-9.66
$\text{C}_4\text{H}_5\text{NO}_4^{2-}$	C_s	B3LYP	UAKS	-511.31958	60.04 (0)	6.19	96.24	-193.69
$\text{HC}_4\text{H}_5\text{NO}_4^-$	C_1	B3LYP	UAKS	-511.99740	67.95 (0)	5.99	93.33	-62.19
$\text{H}_2\text{C}_4\text{H}_5\text{NO}_4$	C_s	B3LYP	UAKS	-512.51258	77.46 (0)	6.36	96.68	-24.53
$\text{C}_4\text{H}_5\text{NO}_4^{2-}$	C_s	B3LYP	Pauling	-511.31958	60.04 (0)	6.19	96.24	-194.77
$\text{HC}_4\text{H}_5\text{NO}_4^-$	C_1	B3LYP	Pauling	-511.99740	67.95 (0)	5.99	93.33	-62.26
$\text{H}_2\text{C}_4\text{H}_5\text{NO}_4$	C_s	B3LYP	Pauling	-512.51258	77.46 (0)	6.36	96.68	-23.87
$\text{C}_4\text{H}_5\text{NO}_4^{2-}$	C_s	B3LYP	Klamt	-511.31958	60.04 (0)	6.19	96.24	-180.79
$\text{HC}_4\text{H}_5\text{NO}_4^-$	C_1	B3LYP	Klamt	-511.99740	67.95 (0)	5.99	93.33	-52.52
$\text{H}_2\text{C}_4\text{H}_5\text{NO}_4$	C_s	B3LYP	Klamt	-512.51258	77.46 (0)	6.36	96.68	-13.65
$\text{C}_4\text{H}_5\text{NO}_4^{2-}$	C_s	B3LYP	SMD	-511.31958	60.04 (0)	6.19	96.24	-191.89
$\text{HC}_4\text{H}_5\text{NO}_4^-$	C_1	B3LYP	SMD	-511.99740	67.95 (0)	5.99	93.33	-60.06
$\text{H}_2\text{C}_4\text{H}_5\text{NO}_4$	C_s	B3LYP	SMD	-512.51258	77.46 (0)	6.36	96.68	-19.63
$\text{C}_4\text{H}_5\text{NO}_4^{2-}$	C_s	PBE	UFF	-510.75819	57.98 (0)	6.30	96.90	-175.66
$\text{HC}_4\text{H}_5\text{NO}_4^-$	C_1	PBE	UFF	-511.43550	64.51 (0)	6.27	97.00	-48.74
$\text{H}_2\text{C}_4\text{H}_5\text{NO}_4$	C_s	PBE	UFF	-511.94703	75.03 (0)	6.44	97.16	-6.32
$\text{C}_4\text{H}_5\text{NO}_4^{2-}$	C_s	PBE	UAKS	-510.75819	57.98 (0)	6.30	96.90	-190.95
$\text{HC}_4\text{H}_5\text{NO}_4^-$	C_1	PBE	UAKS	-511.43550	64.51 (0)	6.27	97.00	-61.25
$\text{H}_2\text{C}_4\text{H}_5\text{NO}_4$	C_s	PBE	UAKS	-511.94703	75.03 (0)	6.44	97.16	-23.85
$\text{C}_4\text{H}_5\text{NO}_4^{2-}$	C_s	PBE	Pauling	-510.75819	57.98 (0)	6.30	96.90	-190.35
$\text{HC}_4\text{H}_5\text{NO}_4^-$	C_1	PBE	Pauling	-511.43550	64.51 (0)	6.27	97.00	-58.89
$\text{H}_2\text{C}_4\text{H}_5\text{NO}_4$	C_s	PBE	Pauling	-511.94703	75.03 (0)	6.44	97.16	-21.44
$\text{C}_4\text{H}_5\text{NO}_4^{2-}$	C_s	PBE	Klamt	-510.75819	57.98 (0)	6.30	96.90	-179.34
$\text{HC}_4\text{H}_5\text{NO}_4^-$	C_1	PBE	Klamt	-511.43550	64.51 (0)	6.27	97.00	-51.12
$\text{H}_2\text{C}_4\text{H}_5\text{NO}_4$	C_s	PBE	Klamt	-511.94703	75.03 (0)	6.44	97.16	-11.68

C ₄ H ₅ NO ₄ ²⁻	C _s	PBE	SMD	-510.75819	57.98 (0)	6.30	96.90	-188.50
HC ₄ H ₅ NO ₄ ⁻	C ₁	PBE	SMD	-511.43550	64.51 (0)	6.27	97.00	-57.81
H ₂ C ₄ H ₅ NO ₄	C _s	PBE	SMD	-511.94703	75.03 (0)	6.44	97.16	-18.11
C ₄ H ₅ NO ₄ ²⁻	C _s	BVP86	UFF	-511.36030	57.89 (0)	6.31	97.01	-176.49
HC ₄ H ₅ NO ₄ ⁻	C ₁	BVP86	UFF	-512.03865	64.48 (0)	6.26	96.94	-49.14
H ₂ C ₄ H ₅ NO ₄	C _s	BVP86	UFF	-512.55110	74.95 (0)	6.45	97.22	-6.43
C ₄ H ₅ NO ₄ ²⁻	C _s	BVP86	UAKS	-511.36030	57.89 (0)	6.31	97.01	-191.87
HC ₄ H ₅ NO ₄ ⁻	C ₁	BVP86	UAKS	-512.03865	64.48 (0)	6.26	96.94	-61.09
H ₂ C ₄ H ₅ NO ₄	C _s	BVP86	UAKS	-512.55110	74.95 (0)	6.45	97.22	-23.73
C ₄ H ₅ NO ₄ ²⁻	C _s	BVP86	Pauling	-511.36030	57.89 (0)	6.31	97.01	-191.50
HC ₄ H ₅ NO ₄ ⁻	C ₁	BVP86	Pauling	-512.03865	64.48 (0)	6.26	96.94	-59.58
H ₂ C ₄ H ₅ NO ₄	C _s	BVP86	Pauling	-512.55110	74.95 (0)	6.45	97.22	-21.65
C ₄ H ₅ NO ₄ ²⁻	C _s	BVP86	Klamt	-511.36030	57.89 (0)	6.31	97.01	-179.49
HC ₄ H ₅ NO ₄ ⁻	C ₁	BVP86	Klamt	-512.03865	64.48 (0)	6.26	96.94	-51.51
H ₂ C ₄ H ₅ NO ₄	C _s	BVP86	Klamt	-512.55110	74.95 (0)	6.45	97.22	-9.56
C ₄ H ₅ NO ₄ ²⁻	C _s	BVP86	SMD	-511.36030	57.89 (0)	6.31	97.01	-189.57
HC ₄ H ₅ NO ₄ ⁻	C ₁	BVP86	SMD	-512.03865	64.48 (0)	6.26	96.94	-58.32
H ₂ C ₄ H ₅ NO ₄	C _s	BVP86	SMD	-512.55110	74.95 (0)	6.45	97.22	-18.23
C ₄ H ₅ NO ₄ ²⁻	C _s	M052X	UFF	-511.26718	61.72 (0)	6.09	95.49	-182.76
HC ₄ H ₅ NO ₄ ⁻	C ₁	M052X	UFF	-511.26096	86.50 (0)	6.76	98.96	-50.68
H ₂ C ₄ H ₅ NO ₄	C _s	M052X	UFF	-512.45762	79.16 (0)	6.28	96.17	-10.77
C ₄ H ₅ NO ₄ ²⁻	C _s	M052X	UAKS	-511.26718	61.72 (0)	6.09	95.49	-198.27
HC ₄ H ₅ NO ₄ ⁻	C ₁	M052X	UAKS	-511.26096	86.50 (0)	6.76	98.96	-62.13
H ₂ C ₄ H ₅ NO ₄	C _s	M052X	UAKS	-512.45762	79.16 (0)	6.28	96.17	-26.22
C ₄ H ₅ NO ₄ ²⁻	C _s	M052X	Pauling	-511.26718	61.72 (0)	6.09	95.49	-200.65
HC ₄ H ₅ NO ₄ ⁻	C ₁	M052X	Pauling	-511.26096	86.50 (0)	6.76	98.96	-60.68
H ₂ C ₄ H ₅ NO ₄	C _s	M052X	Pauling	-512.45762	79.16 (0)	6.28	96.17	-25.11
C ₄ H ₅ NO ₄ ²⁻	C _s	M052X	Klamt	-511.26718	61.72 (0)	6.09	95.49	-184.65
HC ₄ H ₅ NO ₄ ⁻	C ₁	M052X	Klamt	-511.26096	86.50 (0)	6.76	98.96	-53.57
H ₂ C ₄ H ₅ NO ₄	C _s	M052X	Klamt	-512.45762	79.16 (0)	6.28	96.17	-13.85
C ₄ H ₅ NO ₄ ²⁻	C _s	M052X	SMD	-511.26718	61.72 (0)	6.09	95.49	-196.70
HC ₄ H ₅ NO ₄ ⁻	C ₁	M052X	SMD	-511.26096	69.72 (0)	6.76	98.96	-60.80
H ₂ C ₄ H ₅ NO ₄	C _s	M052X	SMD	-512.45762	79.16 (0)	6.28	96.17	-21.02
C ₅ H ₇ NO ₄ ²⁻	C _s	B3LYP	UFF	-550.63401	77.22 (0)	6.95	101.50	-174.92
HC ₅ H ₇ NO ₄ ⁻	C ₁	B3LYP	UFF	-551.31529	84.72 (0)	6.90	99.42	-48.63
H ₂ C ₅ H ₇ NO ₄	C _s	B3LYP	UFF	-551.83209	94.70 (0)	7.15	101.51	-6.66
C ₅ H ₇ NO ₄ ²⁻	C _s	B3LYP	UAKS	-550.63401	77.22 (0)	6.95	101.48	-190.50
HC ₅ H ₇ NO ₄ ⁻	C ₁	B3LYP	UAKS	-551.31529	84.72 (0)	6.90	99.42	-59.89
H ₂ C ₅ H ₇ NO ₄	C _s	B3LYP	UAKS	-551.83209	94.70 (0)	7.15	101.51	-20.16
C ₅ H ₇ NO ₄ ²⁻	C _s	B3LYP	Pauling	-550.63401	77.22 (0)	6.95	101.48	-190.62
HC ₅ H ₇ NO ₄ ⁻	C ₁	B3LYP	Pauling	-551.31529	84.72 (0)	6.90	99.42	-58.97
H ₂ C ₅ H ₇ NO ₄	C _s	B3LYP	Pauling	-551.83209	94.70 (0)	7.15	101.51	-19.08
C ₅ H ₇ NO ₄ ²⁻	C _s	B3LYP	Klamt	-550.63401	77.22 (0)	6.95	101.48	-177.61
HC ₅ H ₇ NO ₄ ⁻	C ₁	B3LYP	Klamt	-551.31529	84.72 (0)	6.90	99.43	-51.65
H ₂ C ₅ H ₇ NO ₄	C _s	B3LYP	Klamt	-551.83209	94.70 (0)	7.15	101.51	-10.69
C ₅ H ₇ NO ₄ ²⁻	C _s	B3LYP	SMD	-550.63401	77.22 (0)	6.95	101.48	-189.73
HC ₅ H ₇ NO ₄ ⁻	C ₁	B3LYP	SMD	-551.31529	84.72 (0)	6.90	99.43	-58.62

$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	B3LYP	SMD	-551.83209	94.70 (0)	7.15	101.51	-18.26
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	PBE	UFF	-550.01612	74.64 (0)	7.07	102.10	-171.95
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	PBE	UFF	-550.69556	81.20 (0)	7.11	100.75	-47.17
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	PBE	UFF	-551.20871	91.72 (0)	7.26	102.13	-3.82
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	PBE	UAKS	-550.01612	74.64 (0)	7.07	102.10	-187.42
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	PBE	UAKS	-550.69556	81.20 (0)	7.11	100.75	-58.46
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	PBE	UAKS	-551.20871	91.72 (0)	7.26	102.13	-19.48
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	PBE	Pauling	-550.01612	74.64 (0)	7.07	102.10	-186.03
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	PBE	Pauling	-550.69556	81.20 (0)	7.11	100.75	-55.63
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	PBE	Pauling	-551.20871	91.72 (0)	7.26	102.13	-16.61
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	PBE	Klamt	-550.01612	74.64 (0)	7.07	102.10	-174.51
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	PBE	Klamt	-550.69556	81.20 (0)	7.11	100.75	-49.87
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	PBE	Klamt	-551.20871	91.72 (0)	7.26	102.13	-7.07
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	PBE	SMD	-550.01612	74.64 (0)	7.07	102.10	-185.82
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	PBE	SMD	-550.69556	81.20 (0)	7.11	100.75	-56.34
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	PBE	SMD	-551.20871	91.72 (0)	7.26	102.13	-16.63
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	BVP86	UFF	-550.67512	74.55 (0)	7.07	102.10	-172.71
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	BVP86	UFF	-551.35567	81.10 (0)	7.13	100.93	-47.53
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	BVP86	UFF	-551.86969	91.64 (0)	7.27	102.22	-3.72
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	BVP86	UAKS	-550.67512	74.55 (0)	7.07	102.10	-188.17
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	BVP86	UAKS	-551.35567	81.10 (0)	7.13	100.93	-58.65
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	BVP86	UAKS	-551.86969	91.64 (0)	7.27	102.22	-19.35
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	BVP86	Pauling	-550.67512	74.55 (0)	7.07	102.10	-187.48
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	BVP86	Pauling	-551.35567	81.10 (0)	7.13	100.93	-56.29
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	BVP86	Pauling	-551.86969	91.64 (0)	7.27	102.22	-16.85
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	BVP86	Klamt	-550.67512	74.55 (0)	7.07	102.10	-175.34
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	BVP86	Klamt	-551.35567	81.10 (0)	7.13	100.93	-50.25
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	BVP86	Klamt	-551.86969	91.64 (0)	7.27	102.22	-7.14
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	BVP86	SMD	-550.67512	74.55 (0)	7.07	102.10	-186.98
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	BVP86	SMD	-551.35567	81.10 (0)	7.13	100.93	-56.86
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	BVP86	SMD	-551.86969	91.64 (0)	7.27	102.22	-16.72
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	M052X	UFF	-550.57799	79.45 (0)	6.76	99.69	-179.41
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	M052X	UFF	-551.22543	87.64 (0)	6.99	101.18	-61.92
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	M052X	UFF	-551.77530	96.85 (0)	7.00	100.27	-7.67
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	M052X	UAKS	-550.57799	79.45 (0)	6.76	99.69	-196.07
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	M052X	UAKS	-551.22543	87.64 (0)	6.99	101.18	-78.94
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	M052X	UAKS	-551.77530	96.85 (0)	7.00	100.27	-21.81
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	M052X	Pauling	-550.57799	79.45 (0)	6.76	99.69	-197.50
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	M052X	Pauling	-551.22543	87.64 (0)	6.99	101.18	-77.08
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	M052X	Pauling	-551.77530	96.85 (0)	7.00	100.27	-20.32
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	M052X	Klamt	-550.57799	79.45 (0)	6.76	99.69	-182.33
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	M052X	Klamt	-551.22543	87.64 (0)	6.99	101.18	-65.47
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	M052X	Klamt	-551.77530	96.85 (0)	7.00	100.27	-10.87
$\text{C}_5\text{H}_7\text{NO}_4^{2-}$	C_s	M052X	SMD	-550.57799	79.45 (0)	6.76	99.69	-195.59
$\text{HC}_5\text{H}_7\text{NO}_4^-$	C_1	M052X	SMD	-551.22543	87.64 (0)	6.99	101.18	-76.12
$\text{H}_2\text{C}_5\text{H}_7\text{NO}_4$	C_s	M052X	SMD	-551.77530	96.85 (0)	7.00	100.27	-19.48
$\text{Fe}(\text{CO})_4^{2-}$	T_d	B3LYP	UFF	-1717.31851	19.60 (0)	6.54	95.44	-171.07

HFe (CO) ₄ ⁻	C _{3v}	B3LYP	UFF	-1718.02018	25.12(0)	6.71	97.67	-33.92
H ₂ Fe (CO) ₄	C _{2v}	B3LYP	UFF	-1718.53458	30.96(0)	6.85	98.33	8.18
Fe (CO) ₄ ²⁻	T _d	B3LYP	UAKS	-1717.31851	19.60(0)	6.54	95.44	-173.68
HFe (CO) ₄ ⁻	C _{3v}	B3LYP	UAKS	-1718.02018	25.12(0)	6.71	97.67	-36.87
H ₂ Fe (CO) ₄	C _{2v}	B3LYP	UAKS	-1718.53458	30.96(0)	6.85	98.33	5.88
Fe (CO) ₄ ²⁻	T _d	B3LYP	Pauling	-1717.31851	19.60(0)	6.54	95.44	-176.58
HFe (CO) ₄ ⁻	C _{3v}	B3LYP	Pauling	-1718.02018	25.12(0)	6.71	97.67	-37.99
H ₂ Fe (CO) ₄	C _{2v}	B3LYP	Pauling	-1718.53458	30.96(0)	6.85	98.33	-2.19
Fe (CO) ₄ ²⁻	T _d	B3LYP	Klamt	-1717.31851	19.60(0)	6.54	95.44	-170.42
HFe (CO) ₄ ⁻	C _{3v}	B3LYP	Klamt	-1718.02018	25.12(0)	6.71	97.67	-34.46
H ₂ Fe (CO) ₄	C _{2v}	B3LYP	Klamt	-1718.53458	30.96(0)	6.85	98.33	7.93
Fe (CO) ₄ ²⁻	T _d	PBE	UFF	-1716.65700	18.99(0)	6.66	96.88	-170.59
HFe (CO) ₄ ⁻	C _{3v}	PBE	UFF	-1717.34756	24.50(0)	6.82	98.73	-33.48
H ₂ Fe (CO) ₄	C _{2v}	PBE	UFF	-1717.85016	30.17(0)	6.94	99.21	8.66
Fe (CO) ₄ ²⁻	T _d	PBE	UAKS	-1716.65700	18.99(0)	6.66	96.88	-173.40
HFe (CO) ₄ ⁻	C _{3v}	PBE	UAKS	-1717.34756	24.50(0)	6.82	98.73	-36.64
H ₂ Fe (CO) ₄	C _{2v}	PBE	UAKS	-1717.85016	30.17(0)	6.94	99.21	6.49
Fe (CO) ₄ ²⁻	T _d	PBE	Pauling	-1716.65700	18.99(0)	6.66	96.88	-175.97
HFe (CO) ₄ ⁻	C _{3v}	PBE	Pauling	-1717.34756	24.50(0)	6.82	98.73	-37.12
H ₂ Fe (CO) ₄	C _{2v}	PBE	Pauling	-1717.85016	30.17(0)	6.94	99.21	0.01
Fe (CO) ₄ ²⁻	T _d	PBE	Klamt	-1716.65700	18.99(0)	6.66	96.88	-170.25
HFe (CO) ₄ ⁻	C _{3v}	PBE	Klamt	-1717.34756	24.50(0)	6.82	98.73	-34.03
H ₂ Fe (CO) ₄	C _{2v}	PBE	Klamt	-1717.85016	30.17(0)	6.94	99.21	8.26
Fe (CO) ₄ ²⁻	T _d	BVP86	UFF	-1717.62208	19.00(0)	6.65	96.67	-170.67
HFe (CO) ₄ ⁻	C _{3v}	BVP86	UFF	-1718.31416	24.50(0)	6.80	98.53	-33.64
H ₂ Fe (CO) ₄	C _{2v}	BVP86	UFF	-1718.81793	30.21(0)	6.92	99.06	8.65
Fe (CO) ₄ ²⁻	T _d	BVP86	UAKS	-1717.62208	19.00(0)	6.65	96.67	-173.68
HFe (CO) ₄ ⁻	C _{3v}	BVP86	UAKS	-1718.31416	24.50(0)	6.80	98.53	-36.78
H ₂ Fe (CO) ₄	C _{2v}	BVP86	UAKS	-1718.81793	30.21(0)	6.92	99.06	6.49
Fe (CO) ₄ ²⁻	T _d	BVP86	Pauling	-1717.62208	19.00(0)	6.65	96.67	-177.02
HFe (CO) ₄ ⁻	C _{3v}	BVP86	Pauling	-1718.31416	24.50(0)	6.80	98.53	-37.38
H ₂ Fe (CO) ₄	C _{2v}	BVP86	Pauling	-1718.81793	30.21(0)	6.92	99.06	-0.07
Fe (CO) ₄ ²⁻	T _d	BVP86	Klamt	-1717.62208	19.00(0)	6.65	96.67	-169.38
HFe (CO) ₄ ⁻	C _{3v}	BVP86	Klamt	-1718.31416	24.50(0)	6.80	98.53	-34.17
H ₂ Fe (CO) ₄	C _{2v}	BVP86	Klamt	-1718.81793	30.21(0)	6.92	99.06	8.26
Fe (CO) ₄ ²⁻	T _d	M052X	UFF	-1717.03509	20.11(0)	6.46	95.10	-174.87
HFe (CO) ₄ ⁻	C _{3v}	M052X	UFF	-1717.74905	25.27(0)	6.74	97.93	-34.90
H ₂ Fe (CO) ₄	C _{2v}	M052X	UFF	-1718.27641	30.97(0)	6.98	99.20	7.47
Fe (CO) ₄ ²⁻	T _d	M052X	UAKS	-1717.03509	20.11(0)	6.46	95.10	-177.37
HFe (CO) ₄ ⁻	C _{3v}	M052X	UAKS	-1717.74905	25.27(0)	6.74	97.93	-37.73
H ₂ Fe (CO) ₄	C _{2v}	M052X	UAKS	-1718.27641	30.97(0)	6.98	99.20	5.53
Fe (CO) ₄ ²⁻	T _d	M052X	Pauling	-1717.03509	20.11(0)	6.46	95.10	-182.12
HFe (CO) ₄ ⁻	C _{3v}	M052X	Pauling	-1717.74905	25.27(0)	6.74	97.93	-39.26
H ₂ Fe (CO) ₄	C _{2v}	M052X	Pauling	-1718.27641	30.97(0)	6.98	99.20	-2.45
Fe (CO) ₄ ²⁻	T _d	M052X	Klamt	-1717.03509	20.11(0)	6.46	95.10	-174.24
HFe (CO) ₄ ⁻	C _{3v}	M052X	Klamt	-1717.74905	25.27(0)	6.74	97.93	-35.40
H ₂ Fe (CO) ₄	C _{2v}	M052X	Klamt	-1718.27641	30.97(0)	6.98	99.20	7.31

Fe (CO) ₄ ²⁻	T _d	M05	UFF	-1717.04526	19.63 (0)	6.62	97.35	-171.44
HFe (CO) ₄ ⁻	C _{3v}	M05	UFF	-1717.74609	24.85 (0)	6.89	99.52	-34.04
H ₂ Fe (CO) ₄	C _{2v}	M05	UFF	-1718.25634	30.44 (0)	7.04	99.92	8.16
Fe (CO) ₄ ²⁻	T _d	M05	UAKS	-1717.04526	19.63 (0)	6.62	97.35	-174.33
HFe (CO) ₄ ⁻	C _{3v}	M05	UAKS	-1717.74609	24.85 (0)	6.89	99.52	-36.98
H ₂ Fe (CO) ₄	C _{2v}	M05	UAKS	-1718.25634	30.44 (0)	7.04	99.92	5.83
Fe (CO) ₄ ²⁻	T _d	M05	Pauling	-1717.04526	19.63 (0)	6.62	97.35	-178.02
HFe (CO) ₄ ⁻	C _{3v}	M05	Pauling	-1717.74609	24.85 (0)	6.89	99.52	-38.30
H ₂ Fe (CO) ₄	C _{2v}	M05	Pauling	-1718.25634	30.44 (0)	7.04	99.92	-1.59
Fe (CO) ₄ ²⁻	T _d	M05	Klamt	-1717.04526	19.63 (0)	6.62	97.35	-171.17
HFe (CO) ₄ ⁻	C _{3v}	M05	Klamt	-1717.74609	24.85 (0)	6.89	99.52	-34.56
H ₂ Fe (CO) ₄	C _{2v}	M05	Klamt	-1718.25634	30.44 (0)	7.04	99.92	7.86
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	B3LYP	UFF	-454.71679	35.18 (0)	5.20	86.48	-186.21
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	B3LYP	UFF	-455.38647	43.09 (0)	5.42	89.58	-55.40
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	B3LYP	UFF	-455.92879	51.76 (0)	5.44	86.98	-2.79
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	B3LYP	UAKS	-454.71679	35.18 (0)	5.20	86.48	-196.75
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	B3LYP	UAKS	-455.38647	43.09 (0)	5.42	89.58	-65.19
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	B3LYP	UAKS	-455.92879	51.76 (0)	5.44	86.98	-12.52
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	B3LYP	Pauling	-454.71679	35.18 (0)	5.20	86.48	-201.58
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	B3LYP	Pauling	-455.38647	43.09 (0)	5.42	89.58	-68.64
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	B3LYP	Pauling	-455.92879	51.76 (0)	5.44	86.98	-17.05
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	B3LYP	Klamt	-454.71679	35.18 (0)	5.20	86.48	-187.92
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	B3LYP	Klamt	-455.38647	43.09 (0)	5.42	89.58	-57.79
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	B3LYP	Klamt	-455.92879	51.76 (0)	5.44	86.98	-5.67
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	B3LYP	SMD	-454.71679	35.18 (0)	5.20	86.48	-196.16
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	B3LYP	SMD	-455.38647	43.09 (0)	5.42	89.58	-63.32
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	B3LYP	SMD	-455.92879	51.76 (0)	5.44	86.98	-10.21
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	PBE	UFF	-454.22689	33.87 (0)	5.34	87.93	-184.00
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	PBE	UFF	-454.89753	41.54 (0)	5.57	91.36	-52.70
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	PBE	UFF	-455.43332	50.11 (0)	5.53	87.51	-1.30
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	PBE	UAKS	-454.22689	33.87 (0)	5.34	87.93	-194.01
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	PBE	UAKS	-454.89753	41.54 (0)	5.57	91.36	-62.27
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	PBE	UAKS	-455.43332	50.11 (0)	5.53	87.51	-12.45
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	PBE	Pauling	-454.22689	33.87 (0)	5.34	87.93	-197.77
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	PBE	Pauling	-454.89753	41.54 (0)	5.57	91.36	-63.99
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	PBE	Pauling	-455.43332	50.11 (0)	5.53	87.51	-14.76
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	PBE	Klamt	-454.22689	33.87 (0)	5.34	87.93	-185.65
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	PBE	Klamt	-454.89753	41.54 (0)	5.57	91.36	-55.00
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	PBE	Klamt	-455.43332	50.11 (0)	5.53	87.51	-3.68
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	PBE	SMD	-454.22689	33.87 (0)	5.34	87.93	-193.43
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	PBE	SMD	-454.89753	41.54 (0)	5.57	91.36	-60.12
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	PBE	SMD	-455.43332	50.11 (0)	5.53	87.51	-9.27
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	BVP86	UFF	-454.75367	33.83 (0)	5.33	87.88	-184.79
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	BVP86	UFF	-455.42518	41.49 (0)	5.57	91.30	-53.04
⁹ H ₂ C ₄ H ₂ O ₄	C _{2h}	BVP86	UFF	-455.96185	50.04 (0)	5.53	87.54	-1.37
⁹ C ₄ H ₂ O ₄ ²⁻	C _{2h}	BVP86	UAKS	-454.75367	33.83 (0)	5.33	87.88	-194.92
⁹ HC ₄ H ₂ O ₄ ⁻	C ₁	BVP86	UAKS	-455.42518	41.49 (0)	5.57	91.30	-62.66

${}^9\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_{2h}	BVP86	UAKS	-455.96185	50.04 (0)	5.53	87.54	-12.47
${}^9\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_{2h}	BVP86	Pauling	-454.75367	33.83 (0)	5.33	87.88	-198.98
${}^9\text{HC}_4\text{H}_2\text{O}_4^-$	C_1	BVP86	Pauling	-455.42518	41.49 (0)	5.57	91.30	-64.66
${}^9\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_{2h}	BVP86	Pauling	-455.96185	50.04 (0)	5.53	87.54	-14.96
${}^9\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_{2h}	BVP86	Klamt	-454.75367	33.83 (0)	5.33	87.88	-186.46
${}^9\text{HC}_4\text{H}_2\text{O}_4^-$	C_1	BVP86	Klamt	-455.42518	41.49 (0)	5.57	91.30	-55.36
${}^9\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_{2h}	BVP86	Klamt	-455.96185	50.04 (0)	5.53	87.54	-4.87
${}^9\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_{2h}	BVP86	SMD	-454.75367	33.83 (0)	5.33	87.88	-194.49
${}^9\text{HC}_4\text{H}_2\text{O}_4^-$	C_1	BVP86	SMD	-455.42518	41.49 (0)	5.57	91.30	-60.65
${}^9\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_{2h}	BVP86	SMD	-455.96185	50.04 (0)	5.53	87.54	-9.41
${}^9\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_{2h}	M052X	UFF	-454.67230	36.24 (0)	5.10	85.30	-188.87
${}^9\text{HC}_4\text{H}_2\text{O}_4^-$	C_1	M052X	UFF	-455.33862	44.32 (0)	5.30	88.29	-58.11
${}^9\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_{2h}	M052X	UFF	-455.87984	52.86 (0)	5.37	86.45	-3.12
${}^9\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_{2h}	M052X	UAKS	-454.67230	36.24 (0)	5.10	85.30	-199.78
${}^9\text{HC}_4\text{H}_2\text{O}_4^-$	C_1	M052X	UAKS	-455.33862	44.32 (0)	5.30	88.29	-67.99
${}^9\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_{2h}	M052X	UAKS	-455.87984	52.86 (0)	5.37	86.45	-13.62
${}^9\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_{2h}	M052X	Pauling	-454.67230	36.24 (0)	5.10	85.30	-206.04
${}^9\text{HC}_4\text{H}_2\text{O}_4^-$	C_1	M052X	Pauling	-455.33862	44.32 (0)	5.30	88.29	-72.80
${}^9\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_{2h}	M052X	Pauling	-455.87984	52.86 (0)	5.37	86.45	-17.98
${}^9\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_{2h}	M052X	Klamt	-454.67230	36.24 (0)	5.10	85.30	-190.65
${}^9\text{HC}_4\text{H}_2\text{O}_4^-$	C_1	M052X	Klamt	-455.33862	44.32 (0)	5.30	88.29	-60.41
${}^9\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_{2h}	M052X	Klamt	-455.87984	52.86 (0)	5.37	86.45	-6.16
${}^9\text{C}_4\text{H}_2\text{O}_4^{2-}$	C_{2h}	M052X	SMD	-454.67230	36.24 (0)	5.10	85.30	-199.76
${}^9\text{HC}_4\text{H}_2\text{O}_4^-$	C_1	M052X	SMD	-455.33862	44.32 (0)	5.30	88.29	-66.51
${}^9\text{H}_2\text{C}_4\text{H}_2\text{O}_4$	C_{2h}	M052X	SMD	-455.87984	52.86 (0)	5.37	86.45	-10.96
$\text{C}_4\text{H}_4\text{O}_4^{2-}$	C_2	B3LYP	UFF	-455.94110	49.48 (0)	5.56	91.14	-185.66
$\text{HC}_4\text{H}_4\text{O}_4^-$	C_1	B3LYP	UFF	-456.63686	56.95 (0)	5.19	86.04	-51.01
$\text{H}_2\text{C}_4\text{H}_4\text{O}_4$	C_1	B3LYP	UFF	-457.15912	66.75 (0)	5.50	88.54	-5.23
$\text{C}_4\text{H}_4\text{O}_4^{2-}$	C_2	B3LYP	UAKS	-455.94110	49.48 (0)	5.56	91.14	-198.61
$\text{HC}_4\text{H}_4\text{O}_4^-$	C_1	B3LYP	UAKS	-456.63686	56.95 (0)	5.19	86.04	-57.18
$\text{H}_2\text{C}_4\text{H}_4\text{O}_4$	C_1	B3LYP	UAKS	-457.15912	66.75 (0)	5.50	88.54	-14.16
$\text{C}_4\text{H}_4\text{O}_4^{2-}$	C_2	B3LYP	Pauling	-455.94110	49.48 (0)	5.56	91.14	-201.91
$\text{HC}_4\text{H}_4\text{O}_4^-$	C_1	B3LYP	Pauling	-456.63686	56.95 (0)	5.19	86.04	-61.43
$\text{H}_2\text{C}_4\text{H}_4\text{O}_4$	C_1	B3LYP	Pauling	-457.15912	66.75 (0)	5.50	88.54	-17.34
$\text{C}_4\text{H}_4\text{O}_4^{2-}$	C_2	B3LYP	Klamt	-455.94110	49.48 (0)	5.56	91.14	-188.31
$\text{HC}_4\text{H}_4\text{O}_4^-$	C_1	B3LYP	Klamt	-456.63686	56.95 (0)	5.19	86.04	-53.19
$\text{H}_2\text{C}_4\text{H}_4\text{O}_4$	C_1	B3LYP	Klamt	-457.15912	66.75 (0)	5.50	88.54	-7.98
$\text{C}_4\text{H}_4\text{O}_4^{2-}$	C_2	B3LYP	SMD	-455.94110	49.48 (0)	5.56	91.14	-197.92
$\text{HC}_4\text{H}_4\text{O}_4^-$	C_1	B3LYP	SMD	-456.63686	56.95 (0)	5.19	86.04	-57.47
$\text{H}_2\text{C}_4\text{H}_4\text{O}_4$	C_1	B3LYP	SMD	-457.15912	66.75 (0)	5.50	88.54	-13.44
$\text{C}_4\text{H}_4\text{O}_4^{2-}$	C_2	PBE	UFF	-455.44070	47.84 (0)	5.65	91.25	-183.35
$\text{HC}_4\text{H}_4\text{O}_4^-$	C_1	PBE	UFF	-456.13699	54.59 (0)	5.31	86.61	-49.39
$\text{H}_2\text{C}_4\text{H}_4\text{O}_4$	C_1	PBE	UFF	-456.65369	64.67 (0)	5.58	89.11	-4.46
$\text{C}_4\text{H}_4\text{O}_4^{2-}$	C_2	PBE	UAKS	-455.44070	47.84 (0)	5.65	91.21	-195.77
$\text{HC}_4\text{H}_4\text{O}_4^-$	C_1	PBE	UAKS	-456.13699	54.59 (0)	5.31	86.61	-55.80
$\text{H}_2\text{C}_4\text{H}_4\text{O}_4$	C_1	PBE	UAKS	-456.65369	64.67 (0)	5.58	89.11	-14.28
$\text{C}_4\text{H}_4\text{O}_4^{2-}$	C_2	PBE	Pauling	-455.44070	47.84 (0)	5.65	91.25	-197.95

HC ₄ H ₄ O ₄ ⁻	C ₁	PBE	Pauling	-456.13699	54.59(0)	5.31	86.61	-58.33
H ₂ C ₄ H ₄ O ₄	C ₁	PBE	Pauling	-456.65369	64.67(0)	5.58	89.11	-15.50
C ₄ H ₄ O ₄ ²⁻	C ₂	PBE	Klamt	-455.44070	47.84(0)	5.65	91.25	-186.04
HC ₄ H ₄ O ₄ ⁻	C ₁	PBE	Klamt	-456.13699	54.59(0)	5.31	86.61	-51.51
H ₂ C ₄ H ₄ O ₄	C ₁	PBE	Klamt	-456.65369	64.67(0)	5.58	89.11	-7.80
C ₄ H ₄ O ₄ ²⁻	C ₂	PBE	SMD	-455.44070	47.84(0)	5.65	91.25	-194.89
HC ₄ H ₄ O ₄ ⁻	C ₁	PBE	SMD	-456.13699	54.59(0)	5.31	86.61	-55.36
H ₂ C ₄ H ₄ O ₄	C ₁	PBE	SMD	-456.65369	64.67(0)	5.58	89.11	-12.47
C ₄ H ₄ O ₄ ²⁻	C ₂	BVP86	UFF	-455.97579	47.79(0)	5.66	91.29	-184.16
HC ₄ H ₄ O ₄ ⁻	C ₁	BVP86	UFF	-456.67304	54.53(0)	5.32	86.64	-49.72
H ₂ C ₄ H ₄ O ₄	C ₁	BVP86	UFF	-457.19050	64.62(0)	5.58	89.10	-4.60
C ₄ H ₄ O ₄ ²⁻	C ₂	BVP86	UAKS	-455.97579	47.79(0)	5.66	91.29	-196.73
HC ₄ H ₄ O ₄ ⁻	C ₁	BVP86	UAKS	-456.67304	54.53(0)	5.32	86.64	-56.08
H ₂ C ₄ H ₄ O ₄	C ₁	BVP86	UAKS	-457.19050	64.62(0)	5.58	89.10	-14.33
C ₄ H ₄ O ₄ ²⁻	C ₂	BVP86	Pauling	-455.97579	47.79(0)	5.66	91.29	-199.21
HC ₄ H ₄ O ₄ ⁻	C ₁	BVP86	Pauling	-456.67304	54.53(0)	5.32	86.64	-59.01
H ₂ C ₄ H ₄ O ₄	C ₁	BVP86	Pauling	-457.19050	64.62(0)	5.58	89.10	-13.05
C ₄ H ₄ O ₄ ²⁻	C ₂	BVP86	Klamt	-455.97579	47.79(0)	5.66	91.29	-186.90
HC ₄ H ₄ O ₄ ⁻	C ₁	BVP86	Klamt	-456.67304	54.53(0)	5.32	86.64	-51.87
H ₂ C ₄ H ₄ O ₄	C ₁	BVP86	Klamt	-457.19050	64.62(0)	5.58	89.10	-7.92
C ₄ H ₄ O ₄ ²⁻	C ₂	BVP86	SMD	-455.97579	47.79(0)	5.66	91.29	-196.01
HC ₄ H ₄ O ₄ ⁻	C ₁	BVP86	SMD	-456.67304	54.53(0)	5.32	86.64	-55.88
H ₂ C ₄ H ₄ O ₄	C ₁	BVP86	SMD	-457.19050	64.62(0)	5.58	89.10	-12.63
C ₄ H ₄ O ₄ ²⁻	C ₂	M052X	UFF	-455.89443	50.74(0)	5.50	90.83	-188.96
HC ₄ H ₄ O ₄ ⁻	C ₁	M052X	UFF	-456.59208	58.13(0)	5.08	85.26	-52.48
H ₂ C ₄ H ₄ O ₄	C ₁	M052X	UFF	-457.11074	68.05(0)	5.45	88.25	-5.53
C ₄ H ₄ O ₄ ²⁻	C ₂	M052X	UAKS	-455.89443	50.74(0)	5.50	90.83	-202.46
HC ₄ H ₄ O ₄ ⁻	C ₁	M052X	UAKS	-456.59208	58.13(0)	5.08	85.26	-58.69
H ₂ C ₄ H ₄ O ₄	C ₁	M052X	UAKS	-457.11074	68.05(0)	5.45	88.25	-15.12
C ₄ H ₄ O ₄ ²⁻	C ₂	M052X	Pauling	-455.89443	50.74(0)	5.50	90.83	-207.14
HC ₄ H ₄ O ₄ ⁻	C ₁	M052X	Pauling	-456.59208	58.13(0)	5.08	85.26	-63.54
H ₂ C ₄ H ₄ O ₄	C ₁	M052X	Pauling	-457.11074	68.05(0)	5.45	88.25	-17.52
C ₄ H ₄ O ₄ ²⁻	C ₂	M052X	Klamt	-455.89443	50.74(0)	5.50	90.83	-191.77
HC ₄ H ₄ O ₄ ⁻	C ₁	M052X	Klamt	-456.59208	58.13(0)	5.08	85.26	-54.71
H ₂ C ₄ H ₄ O ₄	C ₁	M052X	Klamt	-457.11074	68.05(0)	5.45	88.25	-8.96
C ₄ H ₄ O ₄ ²⁻	C ₂	M052X	SMD	-455.89443	50.74(0)	5.50	90.83	-202.39
HC ₄ H ₄ O ₄ ⁻	C ₁	M052X	SMD	-456.59208	58.13(0)	5.08	85.26	-59.22
H ₂ C ₄ H ₄ O ₄	C ₁	M052X	SMD	-457.11074	68.05(0)	5.45	88.25	-14.25

^aPoint group. ^bZero-point energies and number of imaginary frequencies.

^cThermal corrections to 298K. ^dEntropies. ^eFree energy of solvation is the sum of energy difference between gaseous and aqueous state and total non-electrostatic contribution. A correction factor of 1.89 kcal/mol should be added to the calculated values to account for the change of state from 1 mol/atm (24.47 L at 298 K in gas phase) to 1 mol/L (aqueous phase).

^fMaleic acid (D). ^gFumaric acid (N).

Table S2. Point Group, DFT Method, Cavity Model, Total Energies (hartrees), Zero-point Energies (kcal/mol) with number of Imaginary Frequencies in Parentheses, Thermal Corrections (kcal/mol), Entropies (cal/mol·K), and Free energy of Solvation (kcal/mol)

	PG ^a	DFT	Cavity Model	SCF Energy	ZPE ^b (NIF)	TC ^c	S ^d	Solvation Free Energy ^e
^f PO ₄ ³⁻	T _d	B3LYP	UFF	-642.04528	8.58 (0)	3.30	64.56	-526.28
^g HPO ₄ ²⁻	C ₁	B3LYP	UFF	-643.02988	15.80 (0)	3.75	72.13	-234.69
HPO ₄ ²⁻	C ₁	B3LYP	UFF	-643.07253	15.48 (0)	3.83	72.72	-226.04
H ₂ PO ₄ ⁻	C ₁	B3LYP	UFF	-643.80998	23.16 (0)	4.13	74.57	-62.83
H ₃ PO ₄	C ₁	B3LYP	UFF	-644.34250	30.29 (0)	4.53	77.15	-8.37
^f PO ₄ ³⁻	T _d	B3LYP	UAKS	-642.04528	8.58 (0)	3.30	64.56	-528.89
^g HPO ₄ ²⁻	C ₁	B3LYP	UAKS	-643.02988	15.80 (0)	3.75	72.13	-232.24
HPO ₄ ²⁻	C ₁	B3LYP	UAKS	-643.07253	15.48 (0)	3.83	72.72	-225.06
H ₂ PO ₄ ⁻	C ₁	B3LYP	UAKS	-643.80998	23.16 (0)	4.13	74.57	-64.07
H ₃ PO ₄	C ₁	B3LYP	UAKS	-644.34250	30.29 (0)	4.53	77.15	-12.65
^f PO ₄ ³⁻	T _d	B3LYP	Pauling	-642.04528	8.58 (0)	3.30	64.56	-567.94
^g HPO ₄ ²⁻	C ₁	B3LYP	Pauling	-643.02988	15.80 (0)	3.75	72.13	-258.16
HPO ₄ ²⁻	C ₁	B3LYP	Pauling	-643.07253	15.48 (0)	3.83	72.72	-244.82
H ₂ PO ₄ ⁻	C ₁	B3LYP	Pauling	-643.80998	23.16 (0)	4.13	74.57	-75.30
H ₃ PO ₄	C ₁	B3LYP	Pauling	-644.34250	30.29 (0)	4.53	77.15	-21.27
^f PO ₄ ³⁻	T _d	B3LYP	Klamt	-642.04528	8.58 (0)	3.30	64.56	-529.03
^g HPO ₄ ²⁻	C ₁	B3LYP	Klamt	-643.02988	15.80 (0)	3.75	72.14	-236.97
HPO ₄ ²⁻	C ₁	B3LYP	Klamt	-643.07252	15.48 (0)	3.83	72.73	-228.09
H ₂ PO ₄ ⁻	C ₁	B3LYP	Klamt	-643.80998	23.16 (0)	4.12	74.55	-65.33
H ₃ PO ₄	C ₁	B3LYP	Klamt	-644.34250	30.28 (0)	4.53	77.18	-12.01
^f PO ₄ ³⁻	T _d	B3LYP	SMD	-642.04528	8.58 (0)	3.30	64.56	-549.64
^g HPO ₄ ²⁻	C ₁	B3LYP	SMD	-643.02988	15.80 (0)	3.75	72.14	-246.90
HPO ₄ ²⁻	C ₁	B3LYP	SMD	-643.07252	15.48 (0)	3.83	72.73	-235.61
H ₂ PO ₄ ⁻	C ₁	B3LYP	SMD	-643.80998	23.16 (0)	4.12	74.55	-68.51
H ₃ PO ₄	C ₁	B3LYP	SMD	-644.34250	30.28 (0)	4.53	77.18	-15.09
^f PO ₄ ³⁻	T _d	PBE	UFF	-641.56233	8.18 (0)	3.38	65.07	-525.44
^g HPO ₄ ²⁻	C ₁	PBE	UFF	-642.54807	15.18 (0)	3.81	72.52	-233.07
HPO ₄ ²⁻	C ₁	PBE	UFF	-642.59608	14.81 (0)	3.92	73.24	-222.93
H ₂ PO ₄ ⁻	C ₁	PBE	UFF	-643.32928	22.29 (0)	4.23	75.25	-61.39
H ₃ PO ₄	C ₁	PBE	UFF	-643.85834	29.34 (0)	4.62	77.76	-7.71
^f PO ₄ ³⁻	T _d	PBE	UAKS	-641.56233	8.18 (0)	3.38	65.07	-528.01
^g HPO ₄ ²⁻	C ₁	PBE	UAKS	-642.54807	15.18 (0)	3.81	72.52	-230.60
HPO ₄ ²⁻	C ₁	PBE	UAKS	-642.59608	14.81 (0)	3.92	73.24	-222.15
H ₂ PO ₄ ⁻	C ₁	PBE	UAKS	-643.32928	22.29 (0)	4.23	75.25	-62.72
H ₃ PO ₄	C ₁	PBE	UAKS	-643.85834	29.34 (0)	4.62	77.76	-12.29
^f PO ₄ ³⁻	T _d	PBE	Pauling	-641.56233	8.18 (0)	3.38	65.07	-565.84
^g HPO ₄ ²⁻	C ₁	PBE	Pauling	-642.54807	15.18 (0)	3.81	72.52	-255.25
HPO ₄ ²⁻	C ₁	PBE	Pauling	-642.59608	14.81 (0)	3.92	73.24	-240.10
H ₂ PO ₄ ⁻	C ₁	PBE	Pauling	-643.32928	22.29 (0)	4.23	75.25	-72.43

H ₃ PO ₄	C ₁	PBE	Pauling	-643.85834	29.34 (0)	4.62	77.76	-19.62
^f PO ₄ ³⁻	T _d	PBE	Klamt	-641.56234	8.18 (0)	3.38	65.07	-528.09
^g HPO ₄ ²⁻	C ₁	PBE	Klamt	-642.54807	15.18 (0)	3.81	72.52	-235.19
HPO ₄ ²⁻	C ₁	PBE	Klamt	-642.59608	14.81 (0)	3.92	73.24	-224.78
H ₂ PO ₄ ⁻	C ₁	PBE	Klamt	-643.32928	22.29 (0)	4.23	75.21	-63.51
H ₃ PO ₄	C ₁	PBE	Klamt	-643.85834	29.34 (0)	4.62	77.76	-11.24
^f PO ₄ ³⁻	T _d	PBE	SMD	-641.56234	8.18 (0)	3.38	65.07	-548.08
^g HPO ₄ ²⁻	C ₁	PBE	SMD	-642.54807	15.18 (0)	3.81	72.52	-244.57
HPO ₄ ²⁻	C ₁	PBE	SMD	-642.59608	14.81 (0)	3.92	73.24	-231.58
H ₂ PO ₄ ⁻	C ₁	PBE	SMD	-643.32928	22.29 (0)	4.23	75.21	-66.16
H ₃ PO ₄	C ₁	PBE	SMD	-643.85834	29.34 (0)	4.62	77.76	-13.73
^f PO ₄ ³⁻	T _d	BVP86	UFF	-642.09631	8.17 (0)	3.38	65.07	-525.21
^g HPO ₄ ²⁻	C ₁	BVP86	UFF	-643.08032	15.14 (0)	3.82	72.57	-233.13
HPO ₄ ²⁻	C ₁	BVP86	UFF	-643.12402	14.79 (0)	3.92	73.24	-223.90
H ₂ PO ₄ ⁻	C ₁	BVP86	UFF	-643.85816	22.27 (0)	4.23	75.20	-61.81
H ₃ PO ₄	C ₁	BVP86	UFF	-644.38812	29.31 (0)	4.62	77.73	-7.82
^f PO ₄ ³⁻	T _d	BVP86	UAKS	-642.09631	8.17 (0)	3.38	65.07	-527.80
^g HPO ₄ ²⁻	C ₁	BVP86	UAKS	-643.08032	15.14 (0)	3.82	72.57	-230.66
HPO ₄ ²⁻	C ₁	BVP86	UAKS	-643.12402	14.79 (0)	3.92	73.24	-223.02
H ₂ PO ₄ ⁻	C ₁	BVP86	UAKS	-643.85816	22.27 (0)	4.23	75.20	-63.03
H ₃ PO ₄	C ₁	BVP86	UAKS	-644.38812	29.31 (0)	4.62	77.73	-12.35
^f PO ₄ ³⁻	T _d	BVP86	Pauling	-642.09631	8.17 (0)	3.38	65.07	-565.59
^g HPO ₄ ²⁻	C ₁	BVP86	Pauling	-643.08032	15.14 (0)	3.82	72.57	-255.40
HPO ₄ ²⁻	C ₁	BVP86	Pauling	-643.12402	14.79 (0)	3.92	73.24	-241.43
H ₂ PO ₄ ⁻	C ₁	BVP86	Pauling	-643.85816	22.27 (0)	4.23	75.20	-73.10
H ₃ PO ₄	C ₁	BVP86	Pauling	-644.38812	29.31 (0)	4.62	77.73	-19.85
^f PO ₄ ³⁻	T _d	BVP86	Klamt	-642.09631	8.17 (0)	3.38	65.07	-527.87
^g HPO ₄ ²⁻	C ₁	BVP86	Klamt	-643.08032	15.14 (0)	3.82	72.56	-235.27
HPO ₄ ²⁻	C ₁	BVP86	Klamt	-643.12402	14.79 (0)	3.92	73.24	-225.80
H ₂ PO ₄ ⁻	C ₁	BVP86	Klamt	-643.85816	22.27 (0)	4.23	75.24	-63.76
H ₃ PO ₄	C ₁	BVP86	Klamt	-644.38812	29.31 (0)	4.62	77.72	-11.37
^f PO ₄ ³⁻	T _d	BVP86	SMD	-642.09631	8.17 (0)	3.38	65.07	-547.91
^g HPO ₄ ²⁻	C ₁	BVP86	SMD	-643.08032	15.14 (0)	3.82	72.56	-244.71
HPO ₄ ²⁻	C ₁	BVP86	SMD	-643.12402	14.79 (0)	3.92	73.24	-232.78
H ₂ PO ₄ ⁻	C ₁	BVP86	SMD	-643.85816	22.27 (0)	4.23	75.24	-66.76
H ₃ PO ₄	C ₁	BVP86	SMD	-644.38812	29.31 (0)	4.62	77.72	-13.90
^f PO ₄ ³⁻	T _d	M052X	UFF	-642.02662	8.91 (0)	3.24	64.22	-527.03
^g HPO ₄ ²⁻	C ₁	M052X	UFF	-643.00157	16.20 (0)	3.71	71.94	-236.24
HPO ₄ ²⁻	C ₁	M052X	UFF	-643.03359	15.93 (0)	3.78	72.53	-229.86
H ₂ PO ₄ ⁻	C ₁	M052X	UFF	-643.77085	23.67 (0)	4.05	74.07	-64.64
H ₃ PO ₄	C ₁	M052X	UFF	-644.30171	30.67 (0)	4.51	77.15	-9.39
^f PO ₄ ³⁻	T _d	M052X	UAKS	-642.02662	8.91 (0)	3.24	64.22	-529.68
^g HPO ₄ ²⁻	C ₁	M052X	UAKS	-643.00157	16.20 (0)	3.71	71.94	-233.77
HPO ₄ ²⁻	C ₁	M052X	UAKS	-643.03359	15.93 (0)	3.78	72.53	-228.56
H ₂ PO ₄ ⁻	C ₁	M052X	UAKS	-643.77085	23.67 (0)	4.05	74.07	-65.59
H ₃ PO ₄	C ₁	M052X	UAKS	-644.30171	30.67 (0)	4.51	77.15	-13.55

${}^f\text{PO}_4^{3-}$	T_d	M052X	Pauling	-642.02662	8.91(0)	3.24	64.22	-569.56
${}^g\text{HPO}_4^{2-}$	C_1	M052X	Pauling	-643.00157	16.20(0)	3.71	71.94	-260.66
HPO_4^{2-}	C_1	M052X	Pauling	-643.03359	15.93(0)	3.78	72.53	-250.55
H_2PO_4^-	C_1	M052X	Pauling	-643.77085	23.67(0)	4.05	74.07	-78.07
H_3PO_4	C_1	M052X	Pauling	-644.30171	30.67(0)	4.51	77.15	-22.37
${}^f\text{PO}_4^{3-}$	T_d	M052X	Klamt	-642.02662	8.91(0)	3.24	64.23	-530.12
${}^g\text{HPO}_4^{2-}$	C_1	M052X	Klamt	-643.00157	16.20(0)	3.71	71.94	-238.67
HPO_4^{2-}	C_1	M052X	Klamt	-643.03359	15.93(0)	3.78	72.54	-232.05
H_2PO_4^-	C_1	M052X	Klamt	-643.77085	23.68(0)	4.05	74.06	-67.00
H_3PO_4	C_1	M052X	Klamt	-644.30171	30.67(0)	4.51	77.14	-13.16
${}^f\text{PO}_4^{3-}$	T_d	M052X	SMD	-642.02662	8.91(0)	3.24	64.23	-550.95
${}^g\text{HPO}_4^{2-}$	C_1	M052X	SMD	-643.00157	16.20(0)	3.71	71.94	-249.00
HPO_4^{2-}	C_1	M052X	SMD	-643.03359	15.93(0)	3.78	72.54	-240.44
H_2PO_4^-	C_1	M052X	SMD	-643.77085	23.68(0)	4.05	74.06	-70.78
H_3PO_4	C_1	M052X	SMD	-644.30171	30.67(0)	4.51	77.14	-16.36
${}^f\text{AsO}_4^{3-}$	T_d	B3LYP	UFF	-2536.54836	6.72(0)	3.74	68.69	-505.10
${}^g\text{HASO}_4^{2-}$	C_1	B3LYP	UFF	-2537.55828	13.64(0)	4.25	76.76	-222.90
HASO_4^{2-}	C_1	B3LYP	UFF	-2537.51531	13.93(0)	4.15	76.06	-214.36
H_2AsO_4^-	C_1	B3LYP	UFF	-2538.28696	21.03(0)	4.62	79.11	-56.83
H_3AsO_4	C_1	B3LYP	UFF	-2538.81779	27.72(0)	5.36	86.19	-5.43
${}^f\text{AsO}_4^{3-}$	T_d	B3LYP	UAKS	-2536.54836	6.72(0)	3.74	68.69	-516.40
${}^g\text{HASO}_4^{2-}$	C_1	B3LYP	UAKS	-2537.55828	13.64(0)	4.25	76.76	-229.90
HASO_4^{2-}	C_1	B3LYP	UAKS	-2537.51531	13.93(0)	4.15	76.06	-222.14
H_2AsO_4^-	C_1	B3LYP	UAKS	-2538.28696	21.03(0)	4.62	79.11	-65.11
H_3AsO_4	C_1	B3LYP	UAKS	-2538.81779	27.72(0)	5.36	86.19	-15.66
${}^f\text{AsO}_4^{3-}$	T_d	B3LYP	Pauling	-2536.54836	6.72(0)	3.74	68.69	-543.20
${}^g\text{HASO}_4^{2-}$	C_1	B3LYP	Pauling	-2537.55828	13.64(0)	4.25	76.76	-244.90
HASO_4^{2-}	C_1	B3LYP	Pauling	-2537.51531	13.93(0)	4.15	76.06	-232.08
H_2AsO_4^-	C_1	B3LYP	Pauling	-2538.28696	21.03(0)	4.62	79.11	-68.86
H_3AsO_4	C_1	B3LYP	Pauling	-2538.81779	27.72(0)	5.36	86.19	-17.70
${}^f\text{AsO}_4^{3-}$	T_d	B3LYP	Klamt	-2536.54836	6.72(0)	3.74	68.70	-506.90
${}^g\text{HASO}_4^{2-}$	C_1	B3LYP	Klamt	-2537.55828	13.64(0)	4.25	76.76	-224.90
HASO_4^{2-}	C_1	B3LYP	Klamt	-2537.51531	13.93(0)	4.15	76.06	-216.23
H_2AsO_4^-	C_1	B3LYP	Klamt	-2538.28696	21.03(0)	4.62	79.12	-58.82
H_3AsO_4	C_1	B3LYP	Klamt	-2538.81779	27.72(0)	5.36	86.16	-8.51
${}^f\text{AsO}_4^{3-}$	T_d	PBE	UFF	-2535.87351	6.37(0)	3.84	69.35	-504.20
${}^g\text{HASO}_4^{2-}$	C_1	PBE	UFF	-2536.88970	13.07(0)	4.36	77.48	-221.20
HASO_4^{2-}	C_1	PBE	UFF	-2536.84167	13.39(0)	4.23	76.64	-211.49
H_2AsO_4^-	C_1	PBE	UFF	-2537.61438	20.27(0)	4.72	79.87	-54.94
H_3AsO_4	C_1	PBE	UFF	-2538.14256	27.06(0)	5.34	85.04	-4.27
${}^f\text{AsO}_4^{3-}$	T_d	PBE	UAKS	-2535.87351	6.37(0)	3.84	69.35	-514.20
${}^g\text{HASO}_4^{2-}$	C_1	PBE	UAKS	-2536.88970	13.07(0)	4.36	77.48	-227.60
HASO_4^{2-}	C_1	PBE	UAKS	-2536.84167	13.39(0)	4.23	76.64	-218.81
H_2AsO_4^-	C_1	PBE	UAKS	-2537.61438	20.27(0)	4.72	79.87	-63.24
H_3AsO_4	C_1	PBE	UAKS	-2538.14256	27.06(0)	5.34	85.04	-14.98
${}^f\text{AsO}_4^{3-}$	T_d	PBE	Pauling	-2535.87351	6.37(0)	3.84	69.35	-540.70
${}^g\text{HASO}_4^{2-}$	C_1	PBE	Pauling	-2536.88970	13.07(0)	4.36	77.48	-241.70

HAsO ₄ ²⁻	C ₁	PBE	Pauling	-2536.84167	13.39(0)	4.23	76.64	-227.06
H ₂ AsO ₄ ⁻	C ₁	PBE	Pauling	-2537.61438	20.27(0)	4.72	79.87	-65.50
H ₃ AsO ₄	C ₁	PBE	Pauling	-2538.14256	27.06(0)	5.34	85.04	-15.74
^f AsO ₄ ³⁻	T _d	PBE	Klamt	-2535.87355	6.37(0)	3.85	69.38	-505.80
^g HAsO ₄ ²⁻	C ₁	PBE	Klamt	-2536.88970	13.07(0)	4.36	77.47	-223.00
HAsO ₄ ²⁻	C ₁	PBE	Klamt	-2536.84167	13.39(0)	4.23	76.64	-213.19
H ₂ AsO ₄ ⁻	C ₁	PBE	Klamt	-2537.61438	20.28(0)	4.72	79.85	-56.82
H ₃ AsO ₄	C ₁	PBE	Klamt	-2538.14256	27.06(0)	5.34	85.04	-7.23
^f AsO ₄ ³⁻	T _d	BVP86	UFF	-2536.83066	6.33(0)	3.86	69.43	-504.0
^g HAsO ₄ ²⁻	C ₁	BVP86	UFF	-2537.84094	13.04(0)	4.36	77.51	-221.2
HAsO ₄ ²⁻	C ₁	BVP86	UFF	-2537.79724	13.35(0)	4.24	76.71	-212.09
H ₂ AsO ₄ ⁻	C ₁	BVP86	UFF	-2538.56651	20.23(0)	4.73	79.92	-55.31
H ₃ AsO ₄	C ₁	BVP86	UFF	-2539.09445	26.84(0)	5.43	88.35	-4.19
^f AsO ₄ ³⁻	T _d	BVP86	UAKS	-2536.83066	6.33(0)	3.86	69.43	-514.30
^g HAsO ₄ ²⁻	C ₁	BVP86	UAKS	-2537.84094	13.04(0)	4.36	77.51	-227.70
HAsO ₄ ²⁻	C ₁	BVP86	UAKS	-2537.79724	13.35(0)	4.24	76.71	-219.74
H ₂ AsO ₄ ⁻	C ₁	BVP86	UAKS	-2538.56651	20.23(0)	4.73	79.92	-63.58
H ₃ AsO ₄	C ₁	BVP86	UAKS	-2539.09445	26.84(0)	5.44	88.49	-15.07
^f AsO ₄ ³⁻	T _d	BVP86	Pauling	-2536.83066	6.33(0)	3.86	69.43	-540.60
^g HAsO ₄ ²⁻	C ₁	BVP86	Pauling	-2537.84094	13.04(0)	4.36	77.51	-241.80
HAsO ₄ ²⁻	C ₁	BVP86	Pauling	-2537.79724	13.35(0)	4.24	76.71	-228.36
H ₂ AsO ₄ ⁻	C ₁	BVP86	Pauling	-2538.56651	20.23(0)	4.73	79.92	-66.15
H ₃ AsO ₄	C ₁	BVP86	Pauling	-2539.09445	26.84(0)	5.44	88.50	-15.75
^f AsO ₄ ³⁻	T _d	BVP86	Klamt	-2536.83066	6.33(0)	3.86	69.43	-505.50
^g HAsO ₄ ²⁻	C ₁	BVP86	Klamt	-2537.84094	13.04(0)	4.36	77.51	-223.00
HAsO ₄ ²⁻	C ₁	BVP86	Klamt	-2537.79724	13.34(0)	4.24	76.72	-214.11
H ₂ AsO ₄ ⁻	C ₁	BVP86	Klamt	-2538.56651	20.23(0)	4.73	79.91	-57.20
H ₃ AsO ₄	C ₁	BVP86	Klamt	-2539.09445	26.84(0)	5.43	88.36	-7.30
^f AsO ₄ ³⁻	T _d	M052X	UFF	-2536.44668	7.24(0)	3.61	67.90	-506.60
^g HAsO ₄ ²⁻	C ₁	M052X	UFF	-2537.43643	14.34(0)	4.09	75.68	-225.20
HAsO ₄ ²⁻	C ₁	M052X	UFF	-2537.40369	14.53(0)	4.03	75.32	-219.01
H ₂ AsO ₄ ⁻	C ₁	M052X	UFF	-2538.16531	21.77(0)	4.45	77.95	-59.04
H ₃ AsO ₄	C ₁	M052X	UFF	-2538.69550	28.20(0)	5.33	86.92	-6.31
^f AsO ₄ ³⁻	T _d	M052X	UAKS	-2536.44668	7.24(0)	3.61	67.90	-518.90
^g HAsO ₄ ²⁻	C ₁	M052X	UAKS	-2537.43643	14.34(0)	4.09	75.68	-233.00
HAsO ₄ ²⁻	C ₁	M052X	UAKS	-2537.40369	14.53(0)	4.03	75.32	-227.13
H ₂ AsO ₄ ⁻	C ₁	M052X	UAKS	-2538.16531	21.77(0)	4.45	77.95	-67.80
H ₃ AsO ₄	C ₁	M052X	UAKS	-2538.69550	28.20(0)	5.33	86.92	-16.96
^f AsO ₄ ³⁻	T _d	M052X	Pauling	-2536.44668	7.24(0)	3.61	67.90	-546.30
^g HAsO ₄ ²⁻	C ₁	M052X	Pauling	-2537.43643	14.34(0)	4.09	75.68	-248.70
HAsO ₄ ²⁻	C ₁	M052X	Pauling	-2537.40369	14.53(0)	4.03	75.32	-238.91
H ₂ AsO ₄ ⁻	C ₁	M052X	Pauling	-2538.16531	21.77(0)	4.45	77.95	-72.55
H ₃ AsO ₄	C ₁	M052X	Pauling	-2538.69550	28.20(0)	5.33	86.92	-19.02
^f AsO ₄ ³⁻	T _d	M052X	Klamt	-2536.44668	7.24(0)	3.61	67.90	-508.50
^g HAsO ₄ ²⁻	C ₁	M052X	Klamt	-2537.43643	14.35(0)	4.09	75.68	-227.30
HAsO ₄ ²⁻	C ₁	M052X	Klamt	-2537.40369	14.53(0)	4.03	75.32	-221.04

H ₂ AsO ₄ ⁻	C ₁	M052X	Klamt	-2538.16531	21.76 (0)	4.45	77.96	-61.16
H ₃ AsO ₄	C ₁	M052X	Klamt	-2538.69551	28.24 (0)	5.29	85.91	-9.59
^f VO ₄ ³⁻	T _d	B3LYP	UFF	-1244.81570	6.26 (0)	3.95	69.55	-485.45
^g HVO ₄ ²⁻	C ₁	B3LYP	UFF	-1245.76232	13.33 (0)	4.46	78.03	-216.19
HVO ₄ ²⁻	C ₁	B3LYP	UFF	-1245.78414	13.26 (0)	4.45	77.81	-211.93
H ₂ VO ₄ ⁻	C ₁	B3LYP	UFF	-1246.52079	20.27 (0)	4.82	79.91	-54.48
H ₃ VO ₄	C ₁	B3LYP	UFF	-1247.05254	27.39 (0)	5.01	80.63	-1.83
^f VO ₄ ³⁻	T _d	B3LYP	UAKS	-1244.81570	6.26 (0)	3.95	69.55	-507.32
^g HVO ₄ ²⁻	C ₁	B3LYP	UAKS	-1245.76232	13.33 (0)	4.46	78.03	-226.81
HVO ₄ ²⁻	C ₁	B3LYP	UAKS	-1245.78414	13.26 (0)	4.45	77.81	-222.09
H ₂ VO ₄ ⁻	C ₁	B3LYP	UAKS	-1246.52079	20.27 (0)	4.82	79.91	-62.68
H ₃ VO ₄	C ₁	B3LYP	UAKS	-1247.05254	27.39 (0)	5.01	80.63	-11.45
^f VO ₄ ³⁻	T _d	B3LYP	Pauling	-1244.81570	6.26 (0)	3.95	69.55	-519.70
^g HVO ₄ ²⁻	C ₁	B3LYP	Pauling	-1245.76232	13.33 (0)	4.46	78.03	-236.85
HVO ₄ ²⁻	C ₁	B3LYP	Pauling	-1245.78414	13.26 (0)	4.45	77.81	-230.53
H ₂ VO ₄ ⁻	C ₁	B3LYP	Pauling	-1246.52079	20.27 (0)	4.82	79.91	-67.90
H ₃ VO ₄	C ₁	B3LYP	Pauling	-1247.05254	27.39 (0)	5.01	80.63	-17.67
^f VO ₄ ³⁻	T _d	B3LYP	Klamt	-1244.81570	6.26 (0)	3.95	69.55	-489.34
^g HVO ₄ ²⁻	C ₁	B3LYP	Klamt	-1245.76232	13.33 (0)	4.46	78.03	-218.90
HVO ₄ ²⁻	C ₁	B3LYP	Klamt	-1245.78414	13.26 (0)	4.45	77.81	-214.44
H ₂ VO ₄ ⁻	C ₁	B3LYP	Klamt	-1246.52079	20.27 (0)	4.82	79.91	-56.62
H ₃ VO ₄	C ₁	B3LYP	Klamt	-1247.05254	27.39 (0)	5.01	80.63	-4.42
^f VO ₄ ³⁻	T _d	PBE	UFF	-1244.32023	5.81 (0)	4.11	70.59	-480.70
^g HVO ₄ ²⁻	C ₁	PBE	UFF	-1245.25895	12.86 (0)	4.52	78.41	-214.29
HVO ₄ ²⁻	C ₁	PBE	UFF	-1245.28270	12.77 (0)	4.52	78.31	-209.28
H ₂ VO ₄ ⁻	C ₁	PBE	UFF	-1246.01480	19.76 (0)	4.83	79.96	-52.94
H ₃ VO ₄	C ₁	PBE	UFF	-1246.54449	26.59 (0) /	5.11	81.32	-1.18
^f VO ₄ ³⁻	T _d	PBE	UAKS	-1244.32023	5.81 (0)	4.11	70.59	-501.74
^g HVO ₄ ²⁻	C ₁	PBE	UAKS	-1245.25895	12.86 (0)	4.52	78.41	-224.79
HVO ₄ ²⁻	C ₁	PBE	UAKS	-1245.28270	12.77 (0)	4.52	78.31	-219.68
H ₂ VO ₄ ⁻	C ₁	PBE	UAKS	-1246.01480	19.76 (0)	4.83	79.96	-61.89
H ₃ VO ₄	C ₁	PBE	UAKS	-1246.54449	26.59 (0)	5.11	81.32	-11.34
^f VO ₄ ³⁻	T _d	PBE	Pauling	-1244.32023	5.81 (0)	4.11	70.59	-512.62
^g HVO ₄ ²⁻	C ₁	PBE	Pauling	-1245.25895	12.86 (0)	4.52	78.41	-233.25
HVO ₄ ²⁻	C ₁	PBE	Pauling	-1245.28270	12.77 (0)	4.52	78.31	-226.29
H ₂ VO ₄ ⁻	C ₁	PBE	Pauling	-1246.01480	19.76 (0)	4.83	79.96	-65.45
H ₃ VO ₄	C ₁	PBE	Pauling	-1246.54449	26.59 (0)	5.11	81.32	-16.03
^f VO ₄ ³⁻	T _d	PBE	Klamt	-1244.32023	5.81 (0)	4.11	70.59	-484.44
^g HVO ₄ ²⁻	C ₁	PBE	Klamt	-1245.25895	12.86 (0)	4.52	78.41	-216.83
HVO ₄ ²⁻	C ₁	PBE	Klamt	-1245.28270	12.77 (0)	4.52	78.31	-211.94
H ₂ VO ₄ ⁻	C ₁	PBE	Klamt	-1246.01480	19.76 (0)	4.83	79.96	-55.53
H ₃ VO ₄	C ₁	PBE	Klamt	-1246.54449	26.59 (0)	5.11	81.32	-3.54
^f VO ₄ ³⁻	T _d	BVP86	UFF	-1245.02310	5.87 (0)	4.08	70.45	-482.32
^g HVO ₄ ²⁻	C ₁	BVP86	UFF	-1245.96247	12.86 (0)	4.52	78.41	-215.04
HVO ₄ ²⁻	C ₁	BVP86	UFF	-1245.98462	12.78 (0)	4.52	78.26	-210.27
H ₂ VO ₄ ⁻	C ₁	BVP86	UFF	-1246.71741	19.80 (0)	4.80	79.72	-53.33
H ₃ VO ₄	C ₁	BVP86	UFF	-1247.24778	26.24 (0)	5.23	82.18	-1.08

${}^f\text{VO}_4^{3-}$	T_d	BVP86	UAKS	-1245.02310	5.87(0)	4.08	70.45	-503.57
${}^g\text{HVO}_4^{2-}$	C_1	BVP86	UAKS	-1245.96247	12.86(0)	4.52	78.41	-225.64
HVO_4^{2-}	C_1	BVP86	UAKS	-1245.98462	12.78(0)	4.52	78.26	-220.72
H_2VO_4^-	C_1	BVP86	UAKS	-1246.71741	19.80(0)	4.80	79.72	-62.36
H_3VO_4	C_1	BVP86	UAKS	-1247.24778	26.24(0)	5.23	82.18	-11.34
${}^f\text{VO}_4^{3-}$	T_d	BVP86	Pauling	-1245.02310	5.87(0)	4.08	70.45	-227.69
${}^g\text{HVO}_4^{2-}$	C_1	BVP86	Pauling	-1245.96247	12.86(0)	4.52	78.41	-514.65
HVO_4^{2-}	C_1	BVP86	Pauling	-1245.98462	12.78(0)	4.52	78.26	-234.12
H_2VO_4^-	C_1	BVP86	Pauling	-1246.71741	19.80(0)	4.80	79.72	-66.18
H_3VO_4	C_1	BVP86	Pauling	-1247.24778	26.24(0)	5.23	82.18	-16.07
${}^f\text{VO}_4^{3-}$	T_d	BVP86	Klamt	-1245.02310	5.87(0)	4.08	70.45	-486.08
${}^g\text{HVO}_4^{2-}$	C_1	BVP86	Klamt	-1245.96247	12.86(0)	4.52	78.41	-217.60
HVO_4^{2-}	C_1	BVP86	Klamt	-1245.98462	12.78(0)	4.52	78.26	-212.96
H_2VO_4^-	C_1	BVP86	Klamt	-1246.71741	19.80(0)	4.80	79.72	-55.43
H_3VO_4	C_1	BVP86	Klamt	-1247.24778	26.24(0)	5.23	82.18	-3.80
${}^f\text{VO}_4^{3-}$	T_d	M052X	UFF	-1244.65486	6.80(0)	3.79	68.44	-493.27
${}^g\text{HVO}_4^{2-}$	C_1	M052X	UFF	-1245.60439	13.86(0)	4.32	76.99	-219.36
HVO_4^{2-}	C_1	M052X	UFF	-1245.62233	13.75(0)	4.34	77.07	-216.02
H_2VO_4^-	C_1	M052X	UFF	-1246.36080	20.95(0)	4.64	78.57	-55.70
H_3VO_4	C_1	M052X	UFF	-1246.89071	27.86(0)	4.97	80.27	-2.37
${}^f\text{VO}_4^{3-}$	T_d	M052X	UAKS	-1244.65486	6.80(0)	3.79	68.44	-510.97
${}^g\text{HVO}_4^{2-}$	C_1	M052X	UAKS	-1245.60439	13.86(0)	4.32	76.99	-230.39
HVO_4^{2-}	C_1	M052X	UAKS	-1245.62233	13.75(0)	4.34	77.07	-226.78
H_2VO_4^-	C_1	M052X	UAKS	-1246.36080	20.95(0)	4.64	78.57	-64.14
H_3VO_4	C_1	M052X	UAKS	-1246.89071	27.86(0)	4.97	80.27	-12.11
${}^f\text{VO}_4^{3-}$	T_d	M052X	Pauling	-1244.65486	6.80(0)	3.79	68.44	-524.67
${}^g\text{HVO}_4^{2-}$	C_1	M052X	Pauling	-1245.60439	13.86(0)	4.32	76.99	-241.51
HVO_4^{2-}	C_1	M052X	Pauling	-1245.62233	13.75(0)	4.34	77.07	-236.51
H_2VO_4^-	C_1	M052X	Pauling	-1246.36080	20.95(0)	4.64	78.57	-70.22
H_3VO_4	C_1	M052X	Pauling	-1246.89071	27.86(0)	4.97	80.27	-18.64
${}^f\text{VO}_4^{3-}$	T_d	M052X	Klamt	-1244.65486	6.80(0)	3.79	68.44	-497.18
${}^g\text{HVO}_4^{2-}$	C_1	M052X	Klamt	-1245.60439	13.86(0)	4.32	76.99	-222.10
HVO_4^{2-}	C_1	M052X	Klamt	-1245.62233	13.75(0)	4.34	77.07	-218.61
H_2VO_4^-	C_1	M052X	Klamt	-1246.36080	20.95(0)	4.64	78.57	-58.11
H_3VO_4	C_1	M052X	Klamt	-1246.89071	27.86(0)	4.97	80.27	-5.07
${}^f\text{C}_5\text{H}_2\text{NO}_3^{3-}$	C_{2v}	B3LYP	UFF	-471.99272	38.50(0)	4.74	80.34	-436.11
${}^g\text{HC}_5\text{H}_2\text{NO}_3^{2-}$	C_{2v}	B3LYP	UFF	-472.91285	47.37(0)	4.93	81.53	-192.40
$\text{HC}_5\text{H}_2\text{NO}_3^{2-}$	C_{2v}	B3LYP	UFF	-472.94381	47.26(0)	4.93	81.51	-187.39
$\text{H}_2\text{C}_5\text{H}_2\text{NO}_3^-$	C_s	B3LYP	UFF	-473.63940	55.62(0)	5.14	83.88	-52.40
$\text{H}_3\text{C}_5\text{H}_2\text{NO}_3$	C_s	B3LYP	UFF	-474.16500	63.98(0)	5.29	84.60	-7.35
${}^f\text{C}_5\text{H}_2\text{NO}_3^{3-}$	C_{2v}	B3LYP	UAKS	-471.99272	38.50(0)	4.74	80.34	-452.28
${}^g\text{HC}_5\text{H}_2\text{NO}_3^{2-}$	C_{2v}	B3LYP	UAKS	-472.91285	47.37(0)	4.93	81.53	-202.11
$\text{HC}_5\text{H}_2\text{NO}_3^{2-}$	C_{2v}	B3LYP	UAKS	-472.94381	47.26(0)	4.93	81.51	-197.45
$\text{H}_2\text{C}_5\text{H}_2\text{NO}_3^-$	C_s	B3LYP	UAKS	-473.63940	55.62(0)	5.14	83.88	-62.84
$\text{H}_3\text{C}_5\text{H}_2\text{NO}_3$	C_s	B3LYP	UAKS	-474.16500	63.98(0)	5.29	84.60	-20.66
${}^f\text{C}_5\text{H}_2\text{NO}_3^{3-}$	C_{2v}	B3LYP	Pauling	-471.99272	38.50(0)	4.74	80.34	-465.51
${}^g\text{HC}_5\text{H}_2\text{NO}_3^{2-}$	C_{2v}	B3LYP	Pauling	-472.91285	47.37(0)	4.93	81.53	-210.31

HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	B3LYP	Pauling	-472.94381	47.26(0)	4.93	81.51	-202.95
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	B3LYP	Pauling	-473.63940	55.62(0)	5.14	83.88	-63.96
H ₃ C ₅ H ₂ NO ₃	C _s	B3LYP	Pauling	-474.16500	63.98(0)	5.29	84.60	-20.62
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	B3LYP	Klamt	-471.99272	38.50(0)	4.74	80.34	-437.44
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	B3LYP	Klamt	-472.91285	47.37(0)	4.93	81.53	-194.71
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	B3LYP	Klamt	-472.94381	47.26(0)	4.93	81.51	-189.10
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	B3LYP	Klamt	-473.63940	55.62(0)	5.14	83.88	-55.17
H ₃ C ₅ H ₂ NO ₃	C _s	B3LYP	Klamt	-474.16500	63.98(0)	5.29	84.60	-11.40
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	B3LYP	SMD	-471.99272	38.50(0)	4.74	80.34	-455.62
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	B3LYP	SMD	-472.91285	47.37(0)	4.93	81.53	-204.61
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	B3LYP	SMD	-472.94381	47.26(0)	4.93	81.51	-198.31
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	B3LYP	SMD	-473.63940	55.62(0)	5.14	83.88	-60.92
H ₃ C ₅ H ₂ NO ₃	C _s	B3LYP	SMD	-474.16500	63.98(0)	5.29	84.60	-17.27
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	PBE	UFF	-471.47103	37.21(0)	4.88	81.24	-434.31
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	UFF	-472.38868	45.87(0)	5.08	82.56	-191.42
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	UFF	-472.42341	45.76(0)	5.09	82.53	-185.30
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	PBE	UFF	-473.11534	53.92(0)	5.29	84.83	-51.25
H ₃ C ₅ H ₂ NO ₃	C _s	PBE	UFF	-473.63781	62.11(0)	5.44	85.49	-6.60
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	PBE	UAKS	-471.47103	37.21(0)	4.89	81.24	-451.03
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	UAKS	-472.38868	45.87(0)	5.08	82.56	-201.36
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	UAKS	-472.42341	45.76(0)	5.09	82.53	-195.65
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	PBE	UAKS	-473.11534	53.92(0)	5.29	84.83	-62.14
H ₃ C ₅ H ₂ NO ₃	C _s	PBE	UAKS	-473.63781	62.11(0)	5.44	85.49	-20.56
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	PBE	Pauling	-471.47103	37.21(0)	4.88	81.24	-463.45
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	Pauling	-472.38868	45.87(0)	5.08	82.56	-208.51
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	Pauling	-472.42341	45.76(0)	5.09	82.53	-199.73
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	PBE	Pauling	-473.11534	53.92(0)	5.29	84.83	-61.88
H ₃ C ₅ H ₂ NO ₃	C _s	PBE	Pauling	-473.63781	62.11(0)	5.44	85.49	-19.12
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	PBE	Klamt	-471.47103	37.21(0)	4.89	81.24	-435.93
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	Klamt	-472.38868	45.87(0)	5.08	82.56	-193.45
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	Klamt	-472.42341	45.76(0)	5.09	82.53	-187.61
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	PBE	Klamt	-473.11534	53.92(0)	5.29	84.83	-53.97
H ₃ C ₅ H ₂ NO ₃	C _s	PBE	Klamt	-473.63781	62.11(0)	5.44	85.49	-10.62
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	PBE	SMD	-471.47103	37.21(0)	4.89	81.24	-453.84
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	SMD	-472.38868	45.87(0)	5.08	82.56	-203.27
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	PBE	SMD	-472.42341	45.76(0)	5.09	82.53	-195.82
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	PBE	SMD	-473.11534	53.92(0)	5.29	84.83	-59.58
H ₃ C ₅ H ₂ NO ₃	C _s	PBE	SMD	-473.63781	62.11(0)	5.44	85.49	-16.52
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	BVP86	UFF	-472.03715	37.11(0)	4.89	81.28	-434.46
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	UFF	-472.95347	45.76(0)	5.09	82.61	-191.43
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	UFF	-472.98480	45.67(0)	5.09	82.53	-186.12
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	BVP86	UFF	-473.67764	53.83(0)	5.29	84.84	-51.60
H ₃ C ₅ H ₂ NO ₃	C _s	BVP86	UFF	-474.20095	62.00(0)	5.44	85.53	-6.71
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	BVP86	UAKS	-472.03715	37.11(0)	4.89	81.28	-450.93
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	UAKS	-472.95347	45.76(0)	5.09	82.61	-201.47
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	UAKS	-472.98480	45.67(0)	5.09	82.53	-196.37
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	BVP86	UAKS	-473.67764	53.83(0)	5.29	84.84	-62.43

H ₃ C ₅ H ₂ NO ₃	C _s	BVP86	UAKS	-474.20095	62.00(0)	5.44	85.53	-20.60
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	BVP86	Pauling	-472.03715	37.11(0)	4.89	81.28	-463.18
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	Pauling	-472.95347	45.76(0)	5.09	82.61	-208.67
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	Pauling	-472.98480	45.67(0)	5.09	82.53	-200.77
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	BVP86	Pauling	-473.67764	53.83(0)	5.29	84.84	-62.50
H ₃ C ₅ H ₂ NO ₃	C _s	BVP86	Pauling	-474.20095	62.00(0)	5.44	85.53	-19.34
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	BVP86	Klamt	-472.03715	37.11(0)	4.89	81.27	-435.94
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	Klamt	-472.95347	45.76(0)	5.09	82.61	-192.84
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	Klamt	-472.98480	45.67(0)	5.09	82.53	-187.62
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	BVP86	Klamt	-473.67764	53.83(0)	5.29	84.84	-54.32
H ₃ C ₅ H ₂ NO ₃	C _s	BVP86	Klamt	-474.20095	62.00(0)	5.44	85.53	-10.72
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	BVP86	SMD	-472.03715	37.11(0)	4.89	81.27	-453.83
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	SMD	-472.95347	45.76(0)	5.09	82.61	-203.47
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	BVP86	SMD	-472.98480	45.67(0)	5.09	82.53	-196.87
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	BVP86	SMD	-473.67764	53.83(0)	5.29	84.84	-60.07
H ₃ C ₅ H ₂ NO ₃	C _s	BVP86	SMD	-474.20095	62.00(0)	5.44	85.53	-16.65
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	M052X	UFF	-471.96958	39.63(0)	4.66	79.80	-438.44
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	UFF	-472.88071	48.49(0)	4.86	81.07	-194.17
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	UFF	-472.90498	48.40(0)	4.85	81.01	-190.63
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	M052X	UFF	-473.59926	56.78(0)	5.06	83.39	-54.03
H ₃ C ₅ H ₂ NO ₃	C _s	M052X	UFF	-474.12290	65.16(0)	5.23	84.24	-8.32
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	M052X	UAKS	-471.96958	39.63(0)	4.66	79.80	-451.77
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	UAKS	-472.88071	48.49(0)	4.86	81.07	-204.41
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	UAKS	-472.90498	48.40(0)	4.85	81.01	-200.91
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	M052X	UAKS	-473.59926	56.78(0)	5.06	83.39	-64.84
H ₃ C ₅ H ₂ NO ₃	C _s	M052X	UAKS	-474.12290	65.16(0)	5.23	84.24	-21.93
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	M052X	Pauling	-471.96958	39.63(0)	4.66	79.80	-468.93
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	Pauling	-472.88071	48.49(0)	4.86	81.07	-213.41
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	Pauling	-472.90498	48.40(0)	4.85	81.01	-207.74
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	M052X	Pauling	-473.59926	56.78(0)	5.06	83.39	-66.81
H ₃ C ₅ H ₂ NO ₃	C _s	M052X	Pauling	-474.12290	65.16(0)	5.23	84.24	-22.16
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	M052X	Klamt	-471.96958	39.63(0)	4.66	79.80	-439.97
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	Klamt	-472.88071	48.49(0)	4.86	81.07	-195.80
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	Klamt	-472.90498	48.40(0)	4.85	81.01	-192.24
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	M052X	Klamt	-473.59926	56.78(0)	5.06	83.39	-56.90
H ₃ C ₅ H ₂ NO ₃	C _s	M052X	Klamt	-474.12290	65.16(0)	5.23	84.24	-12.52
^f C ₅ H ₂ NO ₃ ³⁻	C _{2v}	M052X	SMD	-471.96958	39.63(0)	4.66	79.80	-458.50
^g HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	SMD	-472.88071	48.49(0)	4.86	81.07	-207.00
HC ₅ H ₂ NO ₃ ²⁻	C _{2v}	M052X	SMD	-472.90498	48.40(0)	4.85	81.01	-202.40
H ₂ C ₅ H ₂ NO ₃ ⁻	C _s	M052X	SMD	-473.59926	56.78(0)	5.06	83.39	-63.19
H ₃ C ₅ H ₂ NO ₃	C _s	M052X	SMD	-474.12290	65.16(0)	5.23	84.24	-18.53
Q_D2 ^h	C _s	B3LYP	UFF	-472.90361	46.52(0)	5.07	83.54	-196.66
Q_D3	C ₁	B3LYP	UFF	-472.89667	46.35(0)	5.10	83.72	-200.27
Q_M2	C _s	B3LYP	UFF	-473.61791	55.30(0)	5.26	84.72	-57.33
Q_M3	C _{2v}	B3LYP	UFF	-473.62107	55.61(0)	5.09	81.99	-52.41
Q_M4	C _s	B3LYP	UFF	-473.60397	54.99(0)	5.27	84.54	-59.83
Q_N2	C _s	B3LYP	UFF	-474.17131	64.12(0)	5.19	83.76	-1.74

Q_N3	C _{2v}	B3LYP	UFF	-474.14958	63.73 (0)	5.43	84.11	-9.85
Q_D2	C _s	B3LYP	UAKS	-472.90361	46.52 (0)	5.07	83.54	-206.48
Q_D3	C ₁	B3LYP	UAKS	-472.89667	46.35 (0)	5.10	83.72	-210.42
Q_M2	C _s	B3LYP	UAKS	-473.61791	55.30 (0)	5.26	84.72	-70.16
Q_M3	C _{2v}	B3LYP	UAKS	-473.62107	55.61 (0)	5.09	81.99	-64.09
Q_M4	C _s	B3LYP	UAKS	-473.60397	54.99 (0)	5.27	84.54	-70.24
Q_N2	C _s	B3LYP	UAKS	-474.17131	64.12 (0)	5.19	83.76	-14.08
Q_N3	C _{2v}	B3LYP	UAKS	-474.14958	63.73 (0)	5.43	84.11	-23.93
Q_D2	C _s	B3LYP	Pauling	-472.90361	46.52 (0)	5.07	83.54	-212.32
Q_D3	C ₁	B3LYP	Pauling	-472.89667	46.35 (0)	5.10	83.72	-216.00
Q_M2	C _s	B3LYP	Pauling	-473.61791	55.30 (0)	5.26	84.72	-70.25
Q_M3	C _{2v}	B3LYP	Pauling	-473.62107	55.61 (0)	5.09	81.99	-62.94
Q_M4	C _s	B3LYP	Pauling	-473.60397	54.99 (0)	5.27	84.54	-71.77
Q_N2	C _s	B3LYP	Pauling	-474.17131	64.12 (0)	5.19	83.76	-13.06
Q_N3	C _{2v}	B3LYP	Pauling	-474.14958	63.73 (0)	5.43	84.11	-23.97
Q_D2	C _s	B3LYP	Klamt	-472.90361	46.52 (0)	5.07	83.54	-198.83
Q_D3	C ₁	B3LYP	Klamt	-472.89667	46.35 (0)	5.10	83.72	-202.24
Q_M2	C _s	B3LYP	Klamt	-473.61791	55.30 (0)	5.26	84.72	-60.18
Q_M3	C _{2v}	B3LYP	Klamt	-473.62107	55.61 (0)	5.09	81.99	-55.03
Q_M4	C _s	B3LYP	Klamt	-473.60397	54.99 (0)	5.27	84.54	-62.56
Q_N2	C _s	B3LYP	Klamt	-474.17131	64.12 (0)	5.19	83.76	-5.35
Q_N3	C _{2v}	B3LYP	Klamt	-474.14958	63.73 (0)	5.43	84.11	-14.05
Q_D2	C _s	PBE	UFF	-472.38501	44.85 (0)	5.29	84.96	-194.00
Q_D3	C ₁	PBE	UFF	-472.36757	44.62 (0)	5.35	85.37	-198.56
Q_M2	C _s	PBE	UFF	-473.09424	53.57 (0)	5.42	85.79	-55.86
Q_M3	C _{2v}	PBE	UFF	-473.09699	53.89 (0)	5.22	82.84	-50.85
Q_M4	C _s	PBE	UFF	-473.08049	53.26 (0)	5.42	85.48	-58.54
Q_N2	C _s	PBE	UFF	-473.64325	62.30 (0)	5.31	84.50	-1.15
Q_N3	C _{2v}	PBE	UFF	-473.62178	61.86 (0)	5.58	85.07	-8.79
Q_D2	C _s	PBE	UAKS	-472.38501	44.85 (0)	5.29	84.96	-204.86
Q_D3	C ₁	PBE	UAKS	-472.36757	44.62 (0)	5.35	85.37	-208.68
Q_M2	C _s	PBE	UAKS	-473.09424	53.57 (0)	5.42	85.79	-68.68
Q_M3	C _{2v}	PBE	UAKS	-473.09699	53.89 (0)	5.22	82.84	-62.79
Q_M4	C _s	PBE	UAKS	-473.08049	53.26 (0)	5.42	85.48	-69.45
Q_N2	C _s	PBE	UAKS	-473.64325	62.30 (0)	5.31	84.50	-13.75
Q_N3	C _{2v}	PBE	UAKS	-473.62178	61.86 (0)	5.58	85.07	-23.87
Q_D2	C _s	PBE	Pauling	-472.38501	44.85 (0)	5.29	84.96	-208.35
Q_D3	C ₁	PBE	Pauling	-472.36757	44.62 (0)	5.35	85.37	-212.95
Q_M2	C _s	PBE	Pauling	-473.09424	53.57 (0)	5.42	85.79	-67.61
Q_M3	C _{2v}	PBE	Pauling	-473.09699	53.89 (0)	5.22	82.84	-61.12
Q_M4	C _s	PBE	Pauling	-473.08049	53.26 (0)	5.42	85.48	-69.48
Q_N2	C _s	PBE	Pauling	-473.64325	62.30 (0)	5.31	84.50	-11.83
Q_N3	C _{2v}	PBE	Pauling	-473.62178	61.86 (0)	5.58	85.07	-22.42
Q_D2	C _s	PBE	Klamt	-472.38501	44.85 (0)	5.29	84.96	-196.02
Q_D3	C ₁	PBE	Klamt	-472.36757	44.62 (0)	5.35	85.37	-200.43
Q_M2	C _s	PBE	Klamt	-473.09424	53.57 (0)	5.42	85.79	-58.82
Q_M3	C _{2v}	PBE	Klamt	-473.09699	53.89 (0)	5.22	82.84	-53.72

Q_M4	C _s	PBE	Klamt	-473.08049	53.26(0)	5.42	85.48	-61.24
Q_N2	C _s	PBE	Klamt	-473.64325	62.30(0)	5.31	84.50	-4.71
Q_N3	C _{2v}	PBE	Klamt	-473.62178	61.86(0)	5.58	85.07	-13.15
Q_D2	C _s	BVP86	UFF	-472.94624	44.85(0)	5.25	84.65	-194.92
Q_D3	C ₁	BVP86	UFF	-472.92986	44.28(0)	5.53	87.36	-199.75
Q_M2	C _s	BVP86	UFF	-473.65654	53.47(0)	5.43	85.84	-56.22
Q_M3	C _{2v}	BVP86	UFF	-473.65938	53.80(0)	5.22	82.84	-51.37
Q_M4	C _s	BVP86	UFF	-473.64278	53.16(0)	5.42	85.51	-58.95
Q_N2	C _s	BVP86	UFF	-474.20647	62.19(0)	5.32	84.53	-1.21
Q_N3	C _{2v}	BVP86	UFF	-474.18493	61.75(0)	5.59	85.13	-9.09
Q_D2	C _s	BVP86	UAKS	-472.94624	44.85(0)	5.25	84.65	-205.81
Q_D3	C ₁	BVP86	UAKS	-472.92986	44.28(0)	5.53	87.35	-209.87
Q_M2	C _s	BVP86	UAKS	-473.65654	53.47(0)	5.43	85.84	-69.09
Q_M3	C _{2v}	BVP86	UAKS	-473.65938	53.80(0)	5.22	82.84	-63.18
Q_M4	C _s	BVP86	UAKS	-473.64278	53.16(0)	5.42	85.51	-69.82
Q_N2	C _s	BVP86	UAKS	-474.20647	62.19(0)	5.32	84.53	-14.06
Q_N3	C _{2v}	BVP86	UAKS	-474.18493	61.75(0)	5.59	85.13	-23.86
Q_D2	C _s	BVP86	Pauling	-472.94624	44.85(0)	5.25	84.65	-209.63
Q_D3	C ₁	BVP86	Pauling	-472.92986	44.28(0)	5.53	87.35	-214.52
Q_M2	C _s	BVP86	Pauling	-473.65654	53.47(0)	5.43	85.84	-68.23
Q_M3	C _{2v}	BVP86	Pauling	-473.65938	53.80(0)	5.22	82.84	-61.59
Q_M4	C _s	BVP86	Pauling	-473.64278	53.16(0)	5.42	85.51	-70.12
Q_N2	C _s	BVP86	Pauling	-474.20647	62.19(0)	5.32	84.53	-11.99
Q_N3	C _{2v}	BVP86	Pauling	-474.18493	61.75(0)	5.59	85.13	-22.67
Q_D2	C _s	BVP86	Klamt	-472.94624	44.85(0)	5.25	84.65	-196.98
Q_D3	C ₁	BVP86	Klamt	-472.92986	44.28(0)	5.52	87.35	-201.61
Q_M2	C _s	BVP86	Klamt	-473.65654	53.47(0)	5.43	85.84	-59.20
Q_M3	C _{2v}	BVP86	Klamt	-473.65938	53.80(0)	5.22	82.84	-54.06
Q_M4	C _s	BVP86	Klamt	-473.64278	53.16(0)	5.42	85.51	-61.66
Q_N2	C _s	BVP86	Klamt	-474.20647	62.19(0)	5.32	84.53	-4.75
Q_N3	C _{2v}	BVP86	Klamt	-474.18493	61.75(0)	5.59	85.13	-13.22
Q_D2	C _s	M052X	UFF	-472.86642	47.78(0)	4.97	82.92	-200.53
Q_D3	C ₁	M052X	UFF	-472.85893	47.48(0)	5.09	83.71	-204.87
Q_M2	C _s	M052X	UFF	-473.57744	56.55(0)	5.16	84.08	-59.39
Q_M3	C _{2v}	M052X	UFF	-473.58409	56.91(0)	5.00	81.44	-53.79
Q_M4	C _s	M052X	UFF	-473.56607	56.25(0)	5.18	84.01	-62.19
Q_N2	C _s	M052X	UFF	-474.13281	65.28(0)	5.13	83.39	-2.58
Q_N3	C _{2v}	M052X	UFF	-474.10786	64.85(0)	5.39	83.85	-10.87
Q_D2	C _s	M052X	UAKS	-472.86642	47.78(0)	4.97	82.92	-210.55
Q_D3	C ₁	M052X	UAKS	-472.85893	47.48(0)	5.09	83.71	-215.21
Q_M2	C _s	M052X	UAKS	-473.57744	56.55(0)	5.16	84.08	-72.61
Q_M3	C _{2v}	M052X	UAKS	-473.58409	56.91(0)	5.00	81.44	-66.32
Q_M4	C _s	M052X	UAKS	-473.56607	56.25(0)	5.18	84.01	-72.88
Q_N2	C _s	M052X	UAKS	-474.13281	65.28(0)	5.13	83.39	-15.16
Q_N3	C _{2v}	M052X	UAKS	-474.10786	64.85(0)	5.39	83.85	-24.83
Q_D2	C _s	M052X	Pauling	-472.86642	47.78(0)	4.97	82.92	-217.74
Q_D3	C ₁	M052X	Pauling	-472.85893	47.48(0)	5.09	83.71	-222.15

Q_M2	C _s	M052X	Pauling	-473.57744	56.55(0)	5.16	84.08	-73.30
Q_M3	C _{2v}	M052X	Pauling	-473.58409	56.91(0)	5.00	81.44	-65.67
Q_M4	C _s	M052X	Pauling	-473.56607	56.25(0)	5.18	84.01	-74.82
Q_N2	C _s	M052X	Pauling	-474.13281	65.28(0)	5.13	83.39	-14.14
Q_N3	C _{2v}	M052X	Pauling	-474.10786	64.85(0)	5.39	83.85	-25.33
Q_D2	C _s	M052X	Klamt	-472.86642	47.78(0)	4.97	82.92	-202.76
Q_D3	C ₁	M052X	Klamt	-472.85893	47.48(0)	5.09	83.71	-206.83
Q_M2	C _s	M052X	Klamt	-473.57744	56.55(0)	5.16	84.08	-62.57
Q_M3	C _{2v}	M052X	Klamt	-473.58409	56.91(0)	5.00	81.44	-56.69
Q_M4	C _s	M052X	Klamt	-473.56607	56.25(0)	5.18	84.01	-65.08
Q_N2	C _s	M052X	Klamt	-474.13281	65.28(0)	5.13	83.39	-6.35
Q_N3	C _{2v}	M052X	Klamt	-474.10786	64.85(0)	5.39	83.85	-15.11

^aPoint group. ^bZero-point energies and number of imaginary frequencies.

^cThermal corrections to 298K. ^dEntropies. ^eFree energy of solvation sum is the energy difference between gaseous and aqueous state and total non-electrostatic contribution. A correction factor of 1.89 kcal/mol should be added to the calculated values to account for the change of state from 1 mol/atm (24.47 L at 298 K in gas phase) to 1 mol/L (aqueous phase).

^fCalculation based on cc-pVTZ basis set. ^gCalculation based on cc-pVTZ basis set. ^hThe series of neutral, monoanion, and dianion isomers based on symbols in Scheme 2.

Table S3. Atomic Radii for Cavity Models

	UFF	UAKS ^a	Pauling	Klamt	SMD
Hydrogen	1.443	1.000	1.200	1.300	1.200
Carbon	1.925	1.500	1.500	2.000	1.850
Nitrogen	1.830	1.500	1.500	1.830	1.890
Oxygen	1.750	1.500	1.400	1.720	1.520
Fluorine	1.682	1.500	1.350	1.720	1.730
Phosphorus	2.074	1.980	1.900	1.800	2.100
Sulfur	2.018	1.980	1.850	2.160	2.490
Vanadium	1.572	2.008	1.572	1.900	
Arsenic	2.115	2.115	2.000	1.900	
Iron	1.456	1.456	1.456	1.900	

^aIn the atom topological model (UATM), the hydrogen atoms are enclosed in the same sphere of the heavy atom they are bound to, and the sphere radii are set according to the atomic number, the charge and the hybridization of the atom, possibly corrected for first neighbor effects. The UAKS values^b are UATM basis radii optimized for PBE0/6-31G(d). The molecular environment modifies the actual radii. ^bBarone, V.; Cossi, M.; Tomasi, J. *J Chem Phys* 1997, 107, 3210.

Table S4. G4MP2 level of theory for free energies (G_{gas}) of $\text{H}_2\text{Fe}(\text{CO})_4$, $\text{H}_1\text{Fe}(\text{CO})_4^-$, and $\text{Fe}(\text{CO})_4^{2-}$ (hartree unit)

Steps	Method	$\text{H}_2\text{Fe}(\text{CO})_4$	$\text{H}_1\text{Fe}(\text{CO})_4^-$	$\text{Fe}(\text{CO})_4^{2-}$
E (CCSD(T))	CCSD(T)/m6-31G(d) ^a	-1715.99603	-1715.46509	-1714.74594
•E (MP2)	MP2/G3MP2LargeXP ^a	-1716.90714	-1716.54064	-1715.97107
	MP2/m6-31G(d) ^a	-1715.93547	-1715.54683	-1714.97090
•E (rel)	CCSD(T)/m6-31G(d) ^a	-1715.99603	-1715.46509	-1714.74594
	CCSD(T)/m6-31G(d)+rel ^a	-1723.32529	-1722.79726	-1722.07780
•E (HF)	HF/3	-1714.53061	-1713.94246	-1713.17675
	HF/4	-1714.56355	-1713.97429	-1713.20742
	Extrapolation	-1714.57157	-1713.98204	-1713.21490
	HF/G3LargeXP	-1714.50112	-1713.91264	-1713.14614
E (HLC)		-0.24780	-0.24780	-0.24780
ZPE	B3LYP/m6-31G(2df,p) ^b	0.04907	0.04017	0.03194
T.C.	B3LYP/m6-31G(2df,p) ^b	0.01088	0.01066	0.01031
-T•S ^c	B3LYP/m6-31G(2df,p) ^b	-0.04650	-0.04635	-0.04491
G(G4MP2)		-1724.60176	-1724.10380	-1723.39720

^aFor MP2 and CCSD(T) level of theory, the number of frozen orbital is 13 (1s,2s,2p orbitals for Fe and 1s orbital for C and O). ^bIn frequency calculation process, scale factor 0.9854 is applied for every thermochemical properties. ^cT=298.15K.