

THE JOURNAL OF
PHYSICAL CHEMISTRY

J. Phys. Chem., 1996, 100(9), 3473-3481, DOI:[10.1021/jp952361k](https://doi.org/10.1021/jp952361k)

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Table S1. Total Energies (hartrees), Spin-Squared Values, and Zero-point Energies (kcal/mol) Using the DFT(Becke3LYP) and MP2/QCI Methods^a

	PG	St	B3LYP/a ^b	B3LYP/b	ZPE (NIF) ^c	MP2/a ^b	QCISD (T) /a	MP2/c
O	K	³ P	-75.06759 (2.00)	-75.09005		-74.88529 (2.01)	-74.90273	-74.92090
O ⁻	K	² P	-75.12722 (0.75)	-75.14920		-74.92525 (0.76)	-74.93937	-74.96771
S	K	³ P	-398.10658 (2.00)	-398.13325		-397.55486 (2.01)	-397.57396	-397.58736
S ⁻	K	² P	-398.18723 (0.75)	-398.21391		-397.60798 (0.76)	-397.62724	-397.65252
O ₂	D _{∞h}	³ Σ _g ⁻	-150.32757 (2.01)	-150.37458	2.35 (0)	-149.95745 (2.05)	-149.97125	-150.04152
O ₂ ⁻	D _{∞h}	² Π _g	-150.34937 (0.76)	-150.39442	1.18 (0)	-149.96121 (0.79)	-149.97812	-150.04792
SO	C _{∞v}	³ Σ ⁻	-473.36058 (2.01)	-473.41691	1.59 (0)	-472.62296 (2.05)	-472.64482	-472.70892
SO ⁻	C _{∞v}	² Π	-473.40700 (0.76)	-473.46089	1.34 (0)	-472.63986 (0.78)	-472.66766	-472.73757
SO ₂	C _{2v}	¹ A ₁	-548.59929	-548.69260	4.19 (0)	-547.69839	-547.71511	-547.84732
SO ₂ ⁻	C _{2v}	² B ₁	-548.65906 (0.75)	-548.74565	3.42 (0)	-547.72942 (0.78)	-547.75210	-547.87878
SO ₂ ²⁻	C _{2v}	¹ A ₁	-548.46413	-548.54387	2.69 (0)	-547.52020	-547.54408	-547.66980
SO ₃	D _{3h}	¹ A ₁ '	-623.77233	-623.89922	7.31 (0)	-622.69086	-622.70986	-622.90466
SO ₃ ⁻	C _{3v}	² A ₁	-623.87109 (0.75)	-623.98960	6.34 (0)	-622.76473 (0.78)	-622.79104	-622.97518
SO ₃ ²⁻	C _{3v}	¹ A ₁	-623.75254	-623.86393	5.70 (0)	-622.63949	-622.66478	-622.84720
SO ₄	C _{2v}	¹ A ₁	-698.87255	-699.02011	9.31 (0)	-697.60937	-697.63844	-697.87091
SO ₄ ⁻	C _{2v}	² B ₁	-699.06630 (0.76)	-699.21443	8.56 (0)	-697.77078 (0.80)	-697.81004	-698.03715
SO ₄ ⁻	D _{2d}	² A ₂	-699.06045 (0.76)	-699.20875	6.59 (2)	-697.77379 (0.83)	-697.80017	-698.03860
SO ₄ ⁻	C _{3v}	² E	-699.06340 (0.76)	-699.21162	7.32 (2)	-697.77110 (0.85)	-697.80508	-698.03609
SO ₄ ²⁻	T _d	¹ A	-699.01040	-699.15307	9.03 (0)	-697.72532	-697.75249	-697.99240
S ₂ O ₃	C _s	¹ A	-1021.90523	-1022.05953	8.38 (0)	-1020.26413	-1020.30314	-1020.52556
S ₂ O ₃ ⁻	C _{3v}	² E	-1022.05502 (0.75)	-1022.20888	7.18 (1)	-1020.39362 (0.76)	-1020.43611	-1020.65810
S ₂ O ₃ ⁻	C _s	² A'	-1022.05615 (0.75)	-1022.20988	7.89 (0)	-1020.39428 (0.76)	-1020.43694	-1020.65892
S ₂ O ₃ ⁻	C _s	² A''	-1022.05562 (0.75)	-1022.20943	7.60 (1)	-1020.39405 (0.76)	-1020.43661	-1020.65862
S ₂ O ₃ ²⁻	C _s	¹ A'	-1022.00324	-1022.15089	7.92 (0)	-1020.33261	-1020.37246	-1020.60102

^aBasis set "a" is 6-31+G(d); basis set "b" is 6-311+G(2d); basis set "c" is 6-31+G(2df).^bSpin-squared value in parentheses.^cZero-point energies with number of imaginary frequencies in parentheses.

Table S2. Total Energies (hartrees), Spin-Squared Values, and Zero-Point Energies (kcal/mol) Using the DFT Method^a

	PG	St	B3LYP/a ^b	B3LYP/b	ZPE (NIF) ^c
SO ₅ ²⁻	C _s	¹ A'	-774.12891	-774.29366	10.20 (1)
SO ₅ ²⁻	C _s	¹ A'	-774.13453	-774.29970	10.54 (0)
SO ₅ ²⁻	C _{4v}	¹ A ₁	-774.03041	-774.19411	8.57 (2)
SO ₅ ²⁻	D _{3h}	¹ A ₁ '	-774.00332	-774.16761	8.23 (1)
SO ₅ ⁻	C _s	² A''	-774.12516 (0.76)	-774.29136	9.70 (1)
SO ₅ ⁻	C _s	² A''	-774.22971 (0.76)	-774.39903	10.87 (0)
SO ₅ ⁻	C _s	² A'	-774.23081 (0.76)	-774.40026	10.98 (0)
S ₂ O ₄ ²⁻	C _{2h}	¹ A _g	-1097.21035	-1097.38568	8.38 (1)
S ₂ O ₄ ²⁻	C ₂	¹ A	-1097.21047	-1097.38554	8.43 (0)
S ₂ O ₄ ²⁻	C _{2v}	¹ A ₁	-1097.20294	-1097.37821	8.12 (1)
S ₂ O ₄ ⁻	C _{2h}	² A _g	-1097.30158 (0.76)	-1097.48356	8.52 (1)
S ₂ O ₄ ⁻	C ₂	² A	-1097.30174 (0.76)	-1097.48275	8.58 (1)
S ₂ O ₄ ⁻	C _{2v}	² A ₁	-1097.29829 (0.76)	-1097.48049	8.44 (1)
S ₂ O ₆ ²⁻	D _{3d}	¹ A _{1g}	-1247.67726	-1247.92009	15.28 (0)
S ₂ O ₆ ²⁻	C _s	¹ A'	-1247.59748	-1247.82207	12.66 (1)
S ₂ O ₆ ⁻	C _s	² A'	-1247.69316 (0.76)	-1247.93393	14.89 (1)
S ₂ O ₆ ⁻	C _s	² A'	-1247.69261 (0.76)	-1247.93333	14.83 (1)
S ₂ O ₆ ⁻	C _s	² A'	-1247.69004 (0.75)	-1247.93202	14.80 (0)
S ₂ O ₆ ⁻	C _s	² A'	-1247.68928 (0.75)	-1247.93136	14.83 (1)
S ₂ O ₆ ⁻	D _{3d}	² A _{1g}	-1247.67677 (0.75)	-1247.92585	14.72 (0)
S ₂ O ₆ ⁻	C _{2h}	² B _g	-1247.64492 (0.77)	-1247.87600	12.33 (1)
S ₂ O ₈ ²⁻	C _{2h}	¹ A _g	-1398.06188	-1398.35252	20.11 (0)
S ₂ O ₈ ⁻	C _{2h}	² B _g	-1398.04214 (0.76)	-1398.33950	19.45 (1)
S ₂ O ₈ ⁻	C _{2h}	² B _g	-1398.04129 (0.76)	-1398.33854	19.47 (1)
H ₂ O	C _{2v}	¹ A ₁	-76.42257	-76.45037	13.24 (0)
SO ₄ ²⁻ · 4H ₂ O	C ₂	¹ A	-1004.85865	-1005.11054	72.42 (0)

^aBasis set "a" is 6-31+G(d); basis set "b" is 6-311+G(2d).^bSpin-squared value in parentheses.^cZero-point energies with number of imaginary frequencies in parentheses.