THE JOURNAL OF
PHYSICAL CHEMISTRY
J. Phys. Chem., 1996, 100(9), 3473-3481, DOI:10.1021/jp952361k

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	^3P	-75.06759(2.00)	-75.09005		-74.88529(2.01)	-74.90273	-74.92090
O^-	K	^2P	-75.12722(0.75)	-75.14920		-74.92525(0.76)	-74.93937	-74.96771
S	K	^3P	-398.10658(2.00)	-398.13325		-397.55486(2.01)	-397.57396	-397.58736
S^-	K	^2P	-398.18723(0.75)	-398.21391		-397.60798(0.76)	-397.62724	-397.65252
O_2	$D_{\infty h}$	$^3\Sigma_g^-$	-150.32757(2.01)	-150.37458	2.35(0)	-149.95745(2.05)	-149.97125	-150.04152
O_2^-	$D_{\infty h}$	$^2\Pi_g$	-150.34937(0.76)	-150.39442	1.18(0)	-149.96121(0.79)	-149.97812	-150.04792
SO	$C_{\infty v}$	$^3\Sigma^-$	-473.36058(2.01)	-473.41691	1.59(0)	-472.62296(2.05)	-472.64482	-472.70892
SO^-	$C_{\infty v}$	$^2\Pi$	-473.40700(0.76)	-473.46089	1.34(0)	-472.63986(0.78)	-472.66766	-472.73757
SO_2	C_{2v}	$^1A_1$	-548.59929	-548.69260	4.19(0)	-547.69839	-547.71511	-547.84732
SO_2^-	C_{2v}	$^2B_1$	-548.65906(0.75)	-548.74565	3.42(0)	-547.72942(0.78)	-547.75210	-547.87878
SO_2^{2-}	C_{2v}	$^1A_1$	-548.46413	-548.54387	2.69(0)	-547.52020	-547.54408	-547.66980
SO_3	D_{3h}	$^1A_1'$	-623.77233	-623.89922	7.31(0)	-622.69086	-622.70986	-622.90466
SO_3^-	C_{3v}	$^2A_1$	-623.87109(0.75)	-623.98960	6.34(0)	-622.76473(0.78)	-622.79104	-622.97518
SO_3^{2-}	C_{3v}	$^1A_1$	-623.75254	-623.86393	5.70(0)	-622.63949	-622.66478	-622.84720
SO_4	C_{2v}	$^1A_1$	-698.87255	-699.02011	9.31(0)	-697.60937	-697.63844	-697.87091
SO_4^-	C_{2v}	$^2B_1$	-699.06630(0.76)	-699.21443	8.56(0)	-697.77078(0.80)	-697.81004	-698.03715
SO_4^-	D_{2d}	$^2A_2$	-699.06045(0.76)	-699.20875	6.59(2)	-697.77379(0.83)	-697.80017	-698.03860
SO_4^-	C_{3v}	^2E	-699.06340(0.76)	-699.21162	7.32(2)	-697.77110(0.85)	-697.80508	-698.03609
SO_4^{2-}	T_d	^1A	-699.01040	-699.15307	9.03(0)	-697.72532	-697.75249	-697.99240
S_2O_3	C_s	^1A	-1021.90523	-1022.05953	8.38(0)	-1020.26413	-1020.30314	-1020.52556
$S_2O_3^-$	C_{3v}	^2E	-1022.05502(0.75)	-1022.20888	7.18(1)	-1020.39362(0.76)	-1020.43611	-1020.65810
$S_2O_3^-$	C_s	$^2A'$	-1022.05615(0.75)	-1022.20988	7.89(0)	-1020.39428(0.76)	-1020.43694	-1020.65892
$S_2O_3^-$	C_s	$^2A"$	-1022.05562(0.75)	-1022.20943	7.60(1)	-1020.39405(0.76)	-1020.43661	-1020.65862
$S_2O_3^{2-}$	C_s	$^1A'$	-1022.00324	-1022.15089	7.92(0)	-1020.33261	-1020.37246	-1020.60102

[a]Basis set "a" is 6-31+G(d); basis set "b" is 6-311+G(2d); basis set "c" is 6-31+G(2df).

[b]Spin-squared value ir parentheses.

[c]Zero-point energies with number of imaginary frequencies in parentheses.

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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	$^1A'$	-774.12891	-774.29366	10.20(1)
SO_5^{2-}	C_s	$^1A'$	-774.13453	-774.29970	10.54(0)
SO_5^{2-}	C_{4v}	$^1A_1$	-774.03041	-774.19411	8.57(2)
SO_5^{2-}	D_{3h}	$^1A_1'$	-774.00332	-774.16761	8.23(1)
SO_5^-	C_s	$^2A"$	-774.12516(0.76)	-774.29136	9.70(1)
SO_5^-	C_s	$^2A"$	-774.22971(0.76)	-774.39903	10.87(0)
SO_5^-	C_s	$^2A'$	-774.23081(0.76)	-774.40026	10.98(0)
$S_2O_4^{2-}$	C_{2h}	^1A_g	-1097.21035	-1097.38568	8.38(1)
$S_2O_4^{2-}$	C_2	^1A	-1097.21047	-1097.38554	8.43(0)
$S_2O_4^{2-}$	C_{2v}	$^1A_1$	-1097.20294	-1097.37821	8.12(1)
$S_2O_4^-$	C_{2h}	^2A_g	-1097.30158(0.76)	-1097.48356	8.52(1)
$S_2O_4^-$	C_2	^2A	-1097.30174(0.76)	-1097.48275	8.58(1)
$S_2O_4^-$	C_{2v}	$^2A_1$	-1097.29829(0.76)	-1097.48049	8.44(1)
$S_2O_6^{2-}$	D_{3d}	$^1A_{1g}$	-1247.67726	-1247.92009	15.28(0)
$S_2O_6^{2-}$	C_s	$^1A'$	-1247.59748	-1247.82207	12.66(1)
$S_2O_6^-$	C_s	$^2A'$	-1247.69316(0.76)	-1247.93393	14.89(1)
$S_2O_6^-$	C_s	$^2A'$	-1247.69261(0.76)	-1247.93333	14.83(1)
$S_2O_6^-$	C_s	$^2A'$	-1247.69004(0.75)	-1247.93202	14.80(0)
$S_2O_6^-$	C_s	$^2A'$	-1247.68928(0.75)	-1247.93136	14.83(1)
$S_2O_6^-$	D_{3d}	$^2A_{1g}$	-1247.67677(0.75)	-1247.92585	14.72(0)
$S_2O_6^-$	C_{2h}	^2B_g	-1247.64492(0.77)	-1247.87600	12.33(1)
$S_2O_8^{2-}$	C_{2h}	^1A_g	-1398.06188	-1398.35252	20.11(0)
$S_2O_8^-$	C_{2h}	^2B_g	-1398.04214(0.76)	-1398.33950	19.45(1)
$S_2O_8^-$	C_{2h}	^2B_g	-1398.04129(0.76)	-1398.33854	19.47(1)
H_2O	C_{2v}	$^1A_1$	-76.42257	-76.45037	13.24(0)
$SO_4^{2-}\cdot 4H_2O$	C_2	^1A	-1004.85865	-1005.11054	72.42(0)

[a]Basis set "a" is 6-31+G(d); basis set "b" is 6-311+G(2d).

[b]Spin-squared value in parentheses.

[c]Zero-point energies with number of imaginary frequencies in parentheses.