ELECTRONIC SUPPLEMENTARY INFORMATION

FOR A PAPER SUBMITTED TO *PHYS. CHEM. CHEM. PHYS.*

Computational simulation and interpretation of the low-lying excited electronic states and electronic spectrum of thioanisole

Shaohong L. Li, Xuefei Xu, and Donald G. Truhlar*

Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota, Minneapolis, Minnesota 55455, USA

Date of preparation: April 24, 2015

Table of contents

Optimized geometries of S_0 and S_1 S-2

Vibrational frequencies of S_0 and S_1 S-4

Optimized geometries of S_0 and S_1

S_0 geometry optimized by DFT–M06-2X/MG3S (in C_s symmetry)

C	-2.146527	-1.006281	0.000000
C	-0.785844	-1.252610	0.000000
C	0.124780	-0.192779	0.000000
C	-0.355566	1.113205	0.000000
C	-1.725347	1.350657	0.000000
C	-2.626371	0.299021	0.000000
H	-2.837318	-1.838612	0.000000
H	-0.417985	-2.270817	0.000000
H	0.323830	1.952522	0.000000
H	-2.083486	2.371455	0.000000
H	-3.690152	0.490180	0.000000
S	1.831544	-0.625646	0.000000
C	2.650283	0.973485	0.000000
H	2.403715	1.543656	-0.892983
H	3.715965	0.759163	0.000000
H	2.403715	1.543656	0.892983

S_0 geometry optimized by CASSCF(12,11)/MB (in C_1 symmetry)

C	-2.170954	-1.014806	0.000001
C	-0.801843	-1.256174	0.000001
C	0.108434	-0.187440	0.000000
C	-0.377264	1.121067	-0.000001
C	-1.756214	1.356922	-0.000001
C	-2.656970	0.296492	0.000000
H	-2.855613	-1.844300	0.000002
H	-0.436769	-2.268134	0.000002
H	0.292006	1.959468	-0.000003
H	-2.115824	2.370740	-0.000002
H	-3.715880	0.482868	-0.000001
S	1.854954	-0.632094	-0.000001
C	2.719519	0.985378	0.000002
H	2.487540	1.555570	0.888892
H	3.774426	0.744637	0.000002
H	2.487540	1.555574	-0.888886

S_0 geometry optimized by PM3 (in C_1 symmetry)

C	-2.154035	-1.013020	0.000009
C	-0.786221	-1.249043	0.000006
C	0.114629	-0.177889	-0.000002
C	-0.377670	1.126799	-0.000006
C	-1.749268	1.358423	-0.000004
C	-2.639688	0.291773	0.000004
H	-2.851936	-1.856830	-0.000007
H	-0.405392	-2.278101	0.000013
H	0.310911	1.980431	-0.000014
H	-2.125359	2.386785	-0.000019
H	-3.718778	0.475898	-0.000029
S	1.819463	-0.618294	-0.000010
C	2.728675	0.936539	0.000015
H	2.535211	1.554248	0.884431
H	3.794736	0.675915	0.000067
H	2.535361	1.554324	-0.884380

S_1 geometry optimized by CASSCF(12,11)/MB (in C_1 symmetry)

C	-2.197732	-1.049166	0.000000
C	-0.783481	-1.295159	0.000001
C	0.132876	-0.188862	0.000000
C	-0.359183	1.162319	-0.000001
C	-1.773277	1.393211	0.000000
C	-2.682285	0.292408	0.000000
H	-2.884671	-1.873524	0.000001
H	-0.408506	-2.300758	0.000001
H	0.312030	1.996005	-0.000001
H	-2.146949	2.399459	-0.000001
H	-3.740347	0.477295	0.000000
S	1.847708	-0.626569	-0.000001
C	2.743148	0.975974	0.000002
H	2.519958	1.547769	0.889270
H	3.792972	0.714726	0.000001
H	2.519958	1.547771	-0.889265

Vibrational frequencies of S_0 and S_1

S_0 frequencies (in cm^{-1}) computed by M06-2X/MG3S at the geometry optimized at the same level

a′					
3237	3227	3213	3204	3196	3170
3073	1660	1643	1526	1496	1482
1365	1348	1304	1214	1177	1129
1118	1061	1017	986	759	710
630	426	337	216		
a″					
3157	1476	1026	1006	975	929
863	765	715	486	414	263
175	49				

S_0 frequencies (in cm^{-1}) computed by CASSCF(12,11)/MB at the geometry optimized at the same level

3377	3358	3346	3334	3327	3294
3291	3205	1724	1705	1623	1616
1604	1565	1481	1446	1307	1280
1187	1161	1153	1098	1053	1041
1029	1008	983	916	856	761
737	713	704	662	492	427
422	333	261	203	177	24

S_0 frequencies (in cm^{-1}) computed by PM3 at the geometry optimized at the same level

3196	3102	3101	3079	3066	3059
3045	3042	1781	1769	1548	1530
1398	1382	1329	1306	1258	1220
1159	1149	1103	1080	1015	998
976	935	927	917	845	765
758	710	637	625	447	422
352	321	195	181	130	60

S_1 frequencies (in cm^{-1}) computed by CASSCF/MB at the geometry optimized at the same level

3401	3376	3364	3357	3347	3305
3296	3211	1811	1652	1629	1616
1604	1547	1501	1478	1401	1253
1245	1123	1057	1024	1013	998
979	736	721	683	631	614
581	554	524	500	394	370
329	263	233	202	121	21