**Singlet-triplet excitation energies of substituted benzenes:
A G4 theoretical study**

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Abstract

Singlet-triplet adiabatic (AE_{S-T}) and well-to-well (WWE_{S-T}) excitation energies of variously substituted phenyl cations were calculated at the G4 level of theory. The G4 E_{S-T} estimates range from 19 to 40 kJ/mol higher than prior density functional theory based predictions for these cations, and suggest that E_{S-T} and ground state multiplicity structure-property trends for phenyl cations previously proposed in the literature may be incorrect. Among the substituents considered, meta-substituted phenyl cations with electron donating groups have singlet ground states, and are not isoenergetic with the corresponding triplet states as previously claimed. Depending on the functional group, ortho- or para-substituted phenyl cations may also be ground state singlets despite the presence of an electron donating moiety.

Keywords: Phenyl cations; Substituent effects; Singlet-triplet excitation energies; Ground state multiplicity

The existence and energetics of aryl cations has long been a topic of substantial interest among the organic chemistry community [1-16]. In particular, the nature of the ground state multiplicity, and magnitude of the singlet-triplet excitation energy (E_{S-T}), for substituted phenyl cations has attracted a modicum of theoretical attention [17-19]. For example, in a recent study, Lazzaroni et al. [17] calculated the E_{S-T} for the parent and variously substituted (o-, m-, and p-CH₃, OCH₃, NH₂, CN, NO₂, SCH₃, and Si(CH₃)₃) phenyl cations at the UB3LYP/6-31G(d) and UB3LYP/6-311++G(2d,p) levels of theory (and subsequently utilized these findings in ref. [20]). The authors reported that "with electron-donating substituents, the triplet is the ground state for ortho and para derivatives, while the two spin states are roughly isoenergetic when the donating group is in the meta position." Other groups have also calculated the E_{S-T} of substituted phenyl cations using density functional theory (DFT) methods [18, 19], and made inferences regarding ground state multiplicities based on the computational results. However, DFT methods, particularly using the B3LYP functional, are known to significantly underestimate the E_{S-T} of organic compounds, and the use of higher-level (e.g., composite) theoretical methods and/or more modern density functionals is required in order to achieve both qualitative and quantitative E_{S-T} predictivity (see, ref. [9, 21-27], and references therein).

In light of these issues, we chose to re-examine the E_{S-T} of several representative substituted phenyl cations using the G4 [28] and G4MP2 [29] composite methods as employed in Gaussian 09 [30]. All calculations were conducted in the gas phase (1 atm) at 298.15 K. Geometries were visualized using Gabedit 2.3.9 [31] and Avogadro 1.01 (<http://avogadro.openmolecules.net/>). Except where noted otherwise, all compounds converged absent imaginary frequencies. The substituents investigated at the o-, m-, and p- positions included the cyano, amino, nitro, thiomethoxy, and methoxy moieties considered by Lazzaroni et al. [17], as well as bromo, chloro, ethynyl, and dimethylamino groups. For the o- and m-methoxy and thiomethoxy substituted phenyl cations, both syn- and anti-conformations are possible in the singlet and triplet states (Figure 1). Based on the geometries presented in their Supporting Information, Lazzaroni et al. [17] appear to have only calculated the energetics of the syn-conformations for these cations. G4 converged geometries with one imaginary frequency are present for the triplet syn-o-methoxyphenyl cation and the singlet anti-o-methoxyphenyl cation, precluding E_{S-T} calculations on these structures. Analogous results were obtained at the G4MP2 level.

At the G4MP2 level, we find the singlet anti-o-thiomethoxyphenyl cation is 0.9 kJ/mol lower in energy than the syn-conformer, equivalent to the G4 energy difference of 1.0 kJ/mol. In contrast, the triplet syn-o-thiomethoxyphenyl cation is 5.4/5.6 (G4MP2/G4) kJ/mol lower in energy than the anti-conformer. Thus, both G4MP2 and G4 calculations suggest the dominant singlet-triplet transition for the o-thiomethoxyphenyl cation would be from an anti-o-thiomethoxyphenyl singlet state to a syn-o-thiomethoxyphenyl triplet state (or vice versa, depending on the ground state of the system). At the G4MP2 level, for the m-thiomethoxyphenyl (singlet syn→anti isomerization enthalpy [$\Delta_{\text{isom}}H^\circ_{(g)}$]=+5.1 kJ/mol; triplet syn→anti $\Delta_{\text{isom}}H^\circ_{(g)}$ =+1.5 kJ/mol) and m-methoxyphenyl (singlet syn→anti $\Delta_{\text{isom}}H^\circ_{(g)}$ =+2.0 kJ/mol; triplet syn→anti $\Delta_{\text{isom}}H^\circ_{(g)}$ =+5.1 kJ/mol) phenyl cations, the syn-conformations are lower in energy than the corresponding anti-geometries. In addition to these substituents, we also conducted G4 E_{S-T} calculations on the p-hydroxy and thiophenyl cations, but the singlet states of both compounds contained one imaginary frequency.

Adiabatic (AE_{S-T}) and well-to-well (WWE_{S-T}) singlet-triplet excitation energies at 298.15 K and 1 atm using the G4 composite method are presented in Table 1 for the parent and substituted phenyl cations under study, along with E_{S-T} data from ref. [17-19]. The G4 values, which are likely more accurate than the previously published DFT results, are systematically higher than the DFT values by 19 to 40

kJ/mol. Of greater import, the G4 E_{S-T} are in qualitative disagreement with the DFT data regarding the ground state multiplicity of some phenyl cations with electron donating substituents. Lazzaroni et al. [17] predicted that the o-, m-, and p-amino and thiomethoxyphenyl cations would all be triplet ground states, whereas the G4 calculations predict only the o- and p-isomers will be triplet ground states, whereas the m-isomers will clearly (+18 kJ/mol for the m-amino and +17 kJ/mol for the m-thiomethoxy) be singlet ground states. Similarly, Lazzaroni et al. [17] predicted the p-methoxyphenyl cation to be a triplet ground state (by almost 20 kJ/mol), while the G4 results predict a singlet ground state (by about 4-6 kJ/mol).

Given the range in E_{S-T} differences between our G4 results and the DFT data of Lazzaroni et al. [17], although neither G4MP2 nor G4 E_{S-T} calculations could be completed on the o-methoxyphenyl cation due to the presence of imaginary frequencies, there is ambiguity regarding the ground state of this cation as well (i.e., the UB3LYP/6-31G(d) E_{S-T} underestimate for the o-methoxyphenyl cation may be greater than 32 kJ/mol, in which case the ground state would be a singlet). Alternatively, the presence of the imaginary frequencies at the G4MP2 and G4 levels may not be artifacts of the computational methods, and these compounds may not exist in the gas phase at ambient temperature for a finite lifetime. Similarly, the presence of G4 level singlet state imaginary frequencies for the p-hydroxy and thiophenyl cations not only prevents comparison with the E_{S-T} estimates for these compounds in ref. [18, 19], but also questions whether they have a gas phase singlet state potential energy well.

As Bondarchuk and Minaev [16] have recently shown at the B3LYP/6-31G (d,p) level of theory, care needs to be taken when investigating phenyl cations via theoretical methods. In this study, the authors show that the singlet o-nitrophenyl cation cannot likely exist in the gas phase, as calculations lead to a rearranged structure. At the G4 level, we are able to reproduce the gas phase findings of Bondarchuk and Minaev [16] for the o-nitrophenyl cation (see Supplementary Material for structure), while the m- and p-nitrophenyl cations give converged structures using the G4 method with no imaginary frequencies and absent any intramolecular rearrangements. However, the triplet states of the o-, m-, and p-nitrophenyl cations all yield one imaginary frequency at the G4 level, preventing comparison with the E_{S-T} estimates of Lazzaroni et al. [17] for these cations (the o-nitrophenyl cation E_{S-T} data was not provided in the Supporting Information of ref. [17], but values of 79.0 and 65.4 kJ/mol for the m- and p- isomers is available from these authors).

In general, the G4 calculations presented herein suggest that the singlet-triplet excitation energy and ground state multiplicity structure-property trends for phenyl cations previously proposed in the literature may be incorrect. It appears that rather than meta-substituted phenyl cations with electron donating groups having approximately isoenergetic singlet and triplet states, it is likely the ground state is clearly a singlet (at least within the confines of the substituents examined herein). Furthermore, not all ortho-/para-substituted phenyl cations with electron donating groups are ground state triplets; in some cases, either the ortho- or para- isomer may be a ground state singlet despite the presence of an electron donating group. In addition, several substituted phenyl cation singlet and/or triplet states may not be minima on their respective potential energy surfaces when examined at higher levels of theory, thereby precluding the formal calculation of singlet-triplet energy gaps.

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123

124 **Appendix A. Supplementary Material**

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126 Supplementary data is associated with this article.

127

128 **Figure Captions**

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130 **Figure 1.** Structures of the syn- and anti-conformations for the o-(thio)methoxyphenyl cations.

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132 **Figures**

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136 Figure 1.

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Table 1. Adiabatic (E_{S-T}) and well-to-well (WWE_{S-T}) singlet-triplet excitation energies at 298.15 K and 1 atm for various substituted phenyl cations using the Gaussian-4 (G4) composite method level of theory. Values are in kJ/mol. Previous E_{S-T} estimates using DFT methods are provided for comparison.

substituent	G4 (current study)						B3LYP/6-311+G**			
	E_{S-T}			WWE_{S-T}			UB3LYP/6-31G(d) ^a [17]		B3LYP/6-31G(d) [18]	
	ortho	meta	para	ortho	meta	para	ortho	meta	para	para
-H	101.7 [27]	101.7[27]	101.7[27]	101.9[27]	101.9[27]	101.9[27]	75.8	75.8	78.7	82.0
-C≡N	78.8	94.6	87.3	79.3	95.0	87.9	43.6	59.3	52.3	n/a ^b
-Br	49.9	63.9	49.2	51.0	65.0	50.4	n/a	n/a	n/a	n/a
-Cl	47.3	66.6	53.1	48.5	67.7	54.1	n/a	n/a	n/a	n/a
-C≡CH	52.4	61.4	46.4	53.4	62.8	47.7	n/a	n/a	n/a	n/a
-NH ₂	-29.4	17.8	-25.4	-27.1	18.4	-23.9	-55.8	-8.7	-45.6	-37.7
-N(CH ₃) ₂	-30.4	18.0	-36.6	-30.2	18.4	-36.0	n/a	n/a	n/a	-54.0
-OH	n/i ^c	n/i	i ^d	n/i	n/i	i ^d	n/a	n/a	-10.9	0.8
-SH	n/i	n/i	i ^d	n/i	n/i	i ^d	n/a	n/a	n/a	-18.0
-SCH ₃	-9.8	16.5	-17.7	-8.7	17.1	-16.6	~-30 ^e	-7.4	n/a	-33.9
-OCH ₃	i ^f	33.7	4.3	i ^f	34.2	5.7	-31.7	10.6	n/a	-10.9

^a The thiomethoxyphenyl cation E_{S-T} in ref. [17] were calculated at the UB3LYP/6-311++G(2d,p) level. ^b not investigated in ref. [17],[18], or [19]. ^c not investigated as part of the current study. ^d singlet structures converged with one imaginary frequency. ^e The energy given for the triplet structure in the Supporting Information from ref. [17] is incorrect, and results in an E_{S-T} of +209.0 kJ/mol. A value of ~-30 kJ/mol was interpolated from Figure 4 in ref. [17]. ^f Triplet structure converged with one imaginary frequency.

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 213

Supplementary Material

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G4 archive entries

¹m-aminophenyl cation

\\1,1\C,0,-3.0628456473,2.990937019,-0.2910219173\C,0,-4.0203558187,2.0432631885,-0.8708644564\C,0,-1.7952297487,2.4870584871,0.146933257\C,0,-1.4881385878,1.1513157382,0.107725841\C,0,-3.5255414109,0.8294086825,-0.7230211998\C,0,-2.4985628546,0.1617027686,-0.2386026425\H,0,-1.0715616574,3.1900372529,0.543944751\H,0,-2.4686118549,-0.8445401251,0.1589965886\H,0,-0.5659132945,0.7816344632,0.5457870241\H,0,-4.7426714392,2.3743771796,-1.6062227865\N,0,-3.2885433196,4.2982614979,-0.4139241195\H,0,-4.2086080471,4.6601615627,-0.6171602872\H,0,-2.5333363194,4.9677322849,-0.3772800526\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-285.7078356\MP4/GTBas1=-285.7952975\CCSD(T)/G3Bas1=-285.7942251\MP2/GTBas2=-285.7189758\MP4/GTBas2=-285.8067298\MP2/GTBas3=-285.911581\MP4/GTBas3=-286.0082052\HF/GTLargeXP=-284.8909403\MP2/GTLargeXP=-286.3250858\HF/GFHFB1=-284.9138173\HF/GFHFB2=-284.9180031\G4=-286.4651771\FreqCoord=-5.7879394607,5.6520518467,-0.5499517224,-7.597371454,3.8612078437,-1.6456953214,-3.3924925707,4.699859417,0.2776636155,-2.8121743786,2.1756714377,0.2035723369,-6.6623077368,1.5673552621,-1.3663120559,-4.7215995209,0.3055739476,-0.4508936488,-2.024958067,6.0282967617,1.0279066108,-4.6650003342,-1.5959495447,0.3004600086,-1.0694211415,1.4770750715,1.0313880024,-8.9623501583,4.4869226055,-3.0353211749,-6.2144462502,8.1225370785,-0.7822032256,-7.9531166098,8.8064290886,-1.1662639229,-4.7873118462,9.38765352,-0.7129559747\PG=C01 [X(C6H6N1)]\NImag=0\\

¹o-aminophenyl cation

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¹p-aminophenyl cation

\\1,1\C,0,-2.893289216,3.0468266551,-0.2793221633\C,0,-4.105428994,2.3091644731,-0.1309934458\C,0,-1.7032529513,2.4061344047,-0.6365413182\C,0,-1.8959080587,1.0723217216,-0.5238323561\C,0,-4.1078137019,0.8991682009,-0.3485576984\C,0,-2.9355623072,0.2270282232,-0.706791673\H,0,-2.8629564909,4.1095431528,-0.0599012994\H,0,-0.7669303484,2.9256020956,-0.7973226282\H,0,-5.008219425,0.3160507674,-0.1821985514\H,0,-2.8930192359,-0.833987415,-0.9185302055\N,0,-5.2405862511,2.9401991483,0.20741

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2493945,-0.3443053639,-5.4670140531,-1.5760078127,-1.7357705333,-9.903
2727903,5.5561711665,0.3919547233,-9.9628632345,7.4468217074,0.6154743
975,-11.5591200156,4.624141419,0.5244798997\PG=C01 [X(C6H6N1)]\NImag=0
\\

¹m-cyanophenyl cation

\\1,1\C,0,-2.9631357077,3.1231851354,-0.5155130535\C,0,-3.9907271466,2
.2148040016,-0.9698565933\C,0,-1.7925952337,2.6153442436,0.0658075322\
C,0,-1.596637707,1.2491342472,0.2160834695\C,0,-3.5290274704,1.0066649
949,-0.6989112567\C,0,-2.556149029,0.2643730128,-0.2025258666\H,0,-1.0
28741983,3.3055829138,0.4029270831\H,0,-2.4269216662,-0.8036961581,-0.
0965214257\H,0,-0.6930901365,0.844511507,0.6653277104\H,0,-4.919043164
2,2.5316960693,-1.4273258722\C,0,-3.2015672136,4.5153973676,-0.6871927
394\N,0,-3.3952635421,5.6483126649,-0.8267389876\\Version=EM64L-G09Rev
B.01\State=1-A\MP2/GTBas1=-322.479414\MP4/GTBas1=-322.5696449\CCSD(T)/
G3Bas1=-322.5626253\MP2/GTBas2=-322.4900235\MP4/GTBas2=-322.5806604\MP
2/GTBas3=-322.6824398\MP4/GTBas3=-322.7818204\HF/GTLargeXP=-321.556981
4\MP2/GTLargeXP=-323.1458096\HF/GFHFB1=-321.5821978\HF/GFHFB2=-321.586
5227\G4=-323.312242\FreqCoord=-5.5995149822,5.9019645681,-0.974178489,
-7.5413813781,4.185373001,-1.8327633495,-3.3875140587,4.9422843637,0.1
243582134,-3.0172079996,2.3605216304,0.4083385792,-6.6688954344,1.9023
21148,-1.3207508664,-4.8304216197,0.4995925912,-0.3827184228,-1.944040
6093,6.2466464167,0.7614218385,-4.5862172951,-1.5187656329,-0.18239906
06,-1.3097505434,1.5958954643,1.2572871612,-9.2956444163,4.7842122226,
-2.6972550008,-6.0500852298,8.5328644059,-1.2986060781,-6.4161182436,1
0.6737640495,-1.56231027\PG=C01 [X(C7H4N1)]\NImag=0\\

¹o-cyanophenyl cation

\\1,1\C,0,-2.7855987682,2.9287826021,-0.3294817141\C,0,-3.765687142,2.
0195843445,-0.2830223207\C,0,-1.6073538728,2.1226740888,-0.5421113148\
C,0,-1.6674307683,0.7396672405,-0.6488310974\C,0,-4.1178837345,0.75295
49332,-0.3439167908\C,0,-2.8761456282,0.0576052879,-0.5552741281\C,0,-
2.7978087127,4.336370724,-0.2117683992\H,0,-0.6800724809,2.6866510996,
-0.6105221568\H,0,-5.0830082715,0.2698885681,-0.2641353151\H,0,-2.9550
925545,-1.0233165126,-0.6347178426\H,0,-0.7518168424,0.1820321445,-0.8
083860874\N,0,-2.7943912239,5.4886054795,-0.117072833\\Version=EM64L-G
09RevB.01\State=1-A\MP2/GTBas1=-322.4717914\MP4/GTBas1=-322.5621758\CC
SD(T)/G3Bas1=-322.5551897\MP2/GTBas2=-322.482275\MP4/GTBas2=-322.57307
17\MP2/GTBas3=-322.6755976\MP4/GTBas3=-322.7751679\HF/GTLargeXP=-321.5
502268\MP2/GTLargeXP=-323.1385338\HF/GFHFB1=-321.5755511\HF/GFHFB2=-32
1.5798885\G4=-323.3050985\FreqCoord=-5.264018788,5.5345970207,-0.62263
02054,-7.1161174005,3.8164613134,-0.5348346757,-3.0374586182,4.0112726
972,-1.0244419185,-3.1509874977,1.397768514,-1.2261130806,-7.781672505
2,1.4228786141,-0.6499085471,-5.4351275557,0.1088582179,-1.0493160307,
-5.2870922392,8.194553079,-0.4001842781,-1.2851507394,5.0770347929,-1.
1537196744,-9.6054935643,0.5100154801,-0.4991434076,-5.5843156253,-1.9

337879561,-1.1994428942,-1.4207279343,0.3439909005,-1.5276283149,-5.28
06341213,10.3719612076,-0.2212355919\PG=C01 [X(C7H4N1)]\NImag=0\

¹p-cyanophenyl cation

\1,1\C,0,-2.7815548718,2.9588453246,0.\C,0,-3.9758042457,2.2226497767
,0.\C,0,-1.5057198316,2.3172756802,0.\C,0,-1.8030474712,1.0286119624,0
.\C,0,-3.9570428613,0.8198441191,0.\C,0,-2.731490144,0.0867768359,0.\C
,0,-5.2288700012,2.9112719939,0.\H,0,-2.7754714043,4.0453264112,0.\H,0
, -0.5573238145,2.8378632771,0.\H,0,-4.8709450074,0.2322544714,0.\H,0,-
2.6625208488,-0.9929037741,0.\N,0,-6.2418995138,3.4679838932,0.\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-322.4799915\MP4/GTBas1=-322
.5699298\CCSD(T)/G3Bas1=-322.5632872\MP2/GTBas2=-322.4907267\MP4/GTBas
2=-322.5810666\MP2/GTBas3=-322.6831941\MP4/GTBas3=-322.7822815\HF/GTLargeXP=-321.5597671\MP2/GTLargeXP=-323.1467824\HF/GFHFB1=-321.5849516\H
F/GFHFB2=-321.5892778\G4=-323.3133451\FreqCoord=-5.2563769313,5.591407
333,0.,-7.5131811823,4.2001993673,0.,-2.8453981146,4.3790164099,0.,-3.
4072659251,1.943794906,0.,-7.4777273039,1.5492808567,0.,-5.1617683069,
0.1639844545,0.,-9.8811322868,5.5015067669,0.,-5.2448808437,7.64455903
52,0.,-1.0531893768,5.3627843963,0.,-9.2047520723,0.4388973441,0.,-5.0
314352273,-1.8763162094,0.,-11.7954806302,6.5535397915,0.\PG=CS [SG(C7
H4N1)]\NImag=0\

¹m-bromophenyl cation

\1,1\C,0,-2.9808830711,2.8769923246,-0.3969639881\C,0,-3.9803078081,
1.9560047394,-0.8684069751\C,0,-1.784970942,2.3994157975,0.1511902439\
C,0,-1.5386718601,1.0376636662,0.2513058293\C,0,-3.4682301857,0.755795
0658,-0.6437633677\C,0,-2.4649570022,0.0298713575,-0.187196843\H,0,-1.
0416872308,3.1039367858,0.5020063993\H,0,-2.2968483197,-1.0347554104,-
0.1202295036\H,0,-0.6133758605,0.6550572172,0.6752901222\H,0,-4.927215
5549,2.2431803876,-1.3033498517\Br,0,-3.3501334487,4.7018480407,-0.549
2492889\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-2802.2697261\M
P4/GTBas1=-2802.345557\CCSD(T)/G3Bas1=-2802.3399081\MP2/GTBas2=-2802.2
786824\MP4/GTBas2=-2802.3548093\MP2/GTBas3=-2802.4642892\MP4/GTBas3=-2
802.5534939\HF/GTLargeXP=-2801.6305824\MP2/GTLargeXP=-2803.9261651\HF/
GFHFB1=-2801.713218\HF/GFHFB2=-2801.7167115\G4=-2804.141581\FreqCoord=
-5.6330526385,5.4367275798,-0.7501532222,-7.521691682,3.6963132721,-1.
6410513549,-3.3731062355,4.5342387362,0.2857081548,-2.907668424,1.9609
001471,0.4748991929,-6.554005217,1.4282456869,-1.2165364587,-4.6580936
635,0.056448685,-0.3537507662,-1.9685035823,5.865590459,0.9486546116,-
4.3404142931,-1.9554043402,-0.2272008349,-1.1591123929,1.2378787418,1.
2761133912,-9.3110879965,4.2389965993,-2.462974275,-6.3308347267,8.885
2051155,-1.0379307347\PG=C01 [X(C6H4Br1)]\NImag=0\

¹o-bromophenyl cation

\1,1\C,0,-2.7237930422,2.6903726842,-0.2928510296\C,0,-3.7101564397,
1.800903546,-0.2104444247\C,0,-1.5433822845,1.877620811,-0.2500359178\
C,0,-1.6103999499,0.4919301015,-0.1445725736\C,0,-4.0747229032,0.53547
18773,-0.1094096773\C,0,-2.8296099234,-0.1766376468,-0.0751679941\H,0,
-0.6020495165,2.4199017083,-0.3055875775\H,0,-5.0496951634,0.070583595
2,-0.059170704\H,0,-2.9084151506,-1.2566775091,0.0074465726\H,0,-0.689
3423708,-0.0782395539,-0.1159804755\Br,0,-2.791023266,4.538320337,-0.4
310468511\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-2802.2632306
\MP4/GTBas1=-2802.3393712\CCSD(T)/G3Bas1=-2802.3342321\MP2/GTBas2=-280
2.2723892\MP4/GTBas2=-2802.3488382\MP2/GTBas3=-2802.4573783\MP4/GTBas3
=-2802.5468802\HF/GTLargeXP=-2801.6269143\MP2/GTLargeXP=-2803.919521\H
F/GFHFB1=-2801.7095186\HF/GFHFB2=-2801.7130423\G4=-2804.1354512\FreqCo
ord=-5.1472228924,5.0840675686,-0.5534082438,-7.0111795812,3.403214493

8,-0.397682329,-2.9165698361,3.5481891141,-0.4724994079,-3.0432148698,
0.9296131684,-0.2732025704,-7.7001103545,1.0118952,-0.2067543264,-5.34
71878181,-0.3337967772,-0.1420469228,-1.1377087046,4.5729514973,-0.577
4768311,-9.5425409133,0.1333836643,-0.1118164256,-5.4961081153,-2.3747
763295,0.0140719828,-1.3026682926,-0.1478513297,-0.2191713355,-5.27426
96032,8.5761825403,-0.814560499\PG=C01 [X(C6H4Br1)]\NImag=0\\

¹p-bromophenyl cation

\\1,1\C,0,-2.8490491285,3.003181546,-0.2320604064\C,0,-4.0254039408,2
.268440059,-0.0592802913\C,0,-1.6320291737,2.3806037471,-0.6530662553\
C,0,-1.9556642739,1.1060731347,-0.7934185018\C,0,-4.0568627138,0.89073
40727,-0.2925924721\C,0,-2.8925558179,0.1759471451,-0.716242337\H,0,-2
.8015401884,4.0736985591,-0.0566823825\H,0,-0.6986482994,2.9061863368,
-0.8002139429\H,0,-4.9590683799,0.3002092937,-0.1648125291\H,0,-2.8678
586021,-0.8877030868,-0.9089233989\Br,0,-5.5902895519,3.1472692723,0.4
957821927\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTbas1=-2802.2671975
\MP4/GTbas1=-2802.342764\CCSD(T)/G3bas1=-2802.3376972\MP2/GTbas2=-2802
.2760938\MP4/GTbas2=-2802.3519599\MP2/GTbas3=-2802.4614768\MP4/GTbas3=
-2802.5504117\HF/GTLargeXP=-2801.6297241\MP2/GTLargeXP=-2803.9232568\H
F/GFHFB1=-2801.7123328\HF/GFHFB2=-2801.7158285\G4=-2804.1392072\FreqCo
ord=-5.3839225919,5.6751906493,-0.4385306144,-7.6069110224,4.286730460
4,-0.1120235156,-3.0840881793,4.4986891129,-1.2341163691,-3.6956698856
,2.0901753076,-1.4993436772,-7.6663594879,1.6832434546,-0.5529196408,-
5.4661383198,0.3324919181,-1.3535018617,-5.2941437064,7.6981746247,-0.
1071141795,-1.320253949,5.4918962678,-1.5121851998,-9.3712811122,0.567
3133477,-0.3114505432,-5.4194673459,-1.6775157213,-1.7176162998,-10.56
41162567,5.9474769911,0.9368925658\PG=C01 [X(C6H4Br1)]\NImag=0\\

¹m-chlorophenyl cation

\\1,1\C,0,-2.9837300757,2.8963031481,-0.3980943592\C,0,-3.9775857843,
1.9704549166,-0.8669838942\C,0,-1.7875440155,2.4156707606,0.1501639981
\C,0,-1.5483919864,1.0536061985,0.2469762386\C,0,-3.4695485046,0.76736
77704,-0.6442520308\C,0,-2.4706060454,0.0373606116,-0.1897502731\H,0,-
1.0436421741,3.1194879393,0.5012642775\H,0,-2.295965148,-1.0257635256,
-0.1197352974\H,0,-0.6238917828,0.6680982921,0.6705808763\H,0,-4.92459
87188,2.2594740756,-1.3019595625\Cl,0,-3.3218162287,4.5629498027,-0.53
7568969\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTbas1=-689.5131519\MP
4/GTbas1=-689.6001337\CCSD(T)/G3bas1=-689.5965857\MP2/GTbas2=-689.5219
166\MP4/GTbas2=-689.6092785\MP2/GTbas3=-689.7198834\MP4/GTbas3=-689.82
12301\HF/GTLargeXP=-688.7435155\MP2/GTLargeXP=-690.4165595\HF/GFHFB1=-
688.7713927\HF/GFHFB2=-688.775863\G4=-690.5922679\FreqCoord=-5.6384326
975,5.4732197478,-0.752289314,-7.5165478023,3.7236201496,-1.6383621217
, -3.3779686399,4.5649561647,0.2837688314,-2.9260368007,1.9910271671,0.
4667174524,-6.5564964785,1.4501149292,-1.2174598988,-4.6687688081,0.07
0601324,-0.3585760499,-1.9721978898,5.8949778801,0.9472522047,-4.33874
53404,-1.9384121405,-0.2262669206,-1.1789846061,1.2625228019,1.2672142
062,-9.306142893,4.2697872073,-2.4603470091,-6.277322936,8.6227254852,
-1.0158581289\PG=C01 [X(C6H4Cl1)]\NImag=0\\

¹o-chlorophenyl cation

\\1,1\C,0,-2.7299537438,2.71096221,-0.2943058314\C,0,-3.7188198953,1.
8151040643,-0.2113774564\C,0,-1.55403686,1.8905555429,-0.2508437547\C,
0,-1.6128249098,0.5058260196,-0.145583641\C,0,-4.0714640785,0.54666634
9,-0.1103007905\C,0,-2.8286057874,-0.1678941234,-0.0758439131\H,0,-0.6
170446958,2.4416092218,-0.3069866929\H,0,-5.0465746096,0.080764092,-0.
0599853143\H,0,-2.9069014483,-1.247804582,0.0067490542\H,0,-0.68818621
75,-0.0585470498,-0.1174862385\Cl,0,-2.7581777478,4.3963182859,-0.4208

550192\\Version=EM64L-G09RevB.01\\State=1-A\\MP2/GTbas1=-689.5037357\\MP4/GTbas1=-689.5911706\\CCSD(T)/G3Bas1=-689.5880292\\MP2/GTbas2=-689.5124302\\MP4/GTbas2=-689.6002515\\MP2/GTbas3=-689.7095837\\MP4/GTbas3=-689.8114853\\HF/GTLargeXP=-688.7361924\\MP2/GTLargeXP=-690.4065312\\HF/GFHFB1=-688.7640215\\HF/GFHFB2=-688.768557\\G4=-690.5830335\\FreqCoord=-5.1588649311,5.1229761336,-0.5561574207,-7.0275511396,3.4300495842,-0.3994455032,-2.9367040658,3.5726322151,-0.4740259986,-3.0477973798,0.9558726479,-0.2751132109,-7.6939520683,1.0330496856,-0.2084382864,-5.345290276,-0.3172739126,-0.1433242246,-1.1660454867,4.6139727528,-0.5801207759,-9.5366439213,0.1526220153,-0.113355816,-5.4932476325,-2.3580089274,0.0127538641,-1.3004834796,-0.11063789,-0.2220168152,-5.2122005692,8.3078375533,-0.7953007279\\PG=C01 [X(C6H4Cl1)]\\NImag=0\\

¹p-chlorophenyl cation

\\1,1\\C,0,-2.8586224968,3.0113284086,-0.2281797026\\C,0,-4.0352168418,2.273947849,-0.0557992479\\C,0,-1.6439228849,2.3885315994,-0.6486308536\\C,0,-1.9696192161,1.113912305,-0.7884633059\\C,0,-4.0688394378,0.8946786351,-0.288829974\\C,0,-2.905534641,0.1819910301,-0.7118582154\\H,0,-2.8187848864,4.0818337509,-0.0508367334\\H,0,-0.7089217273,2.911230555,-0.7967030314\\H,0,-4.9749783674,0.3106851311,-0.1588946522\\H,0,-2.8774902988,-0.8815542698,-0.9053813678\\Cl,0,-5.4670392315,3.0780544675,0.4520678521\\Version=EM64L-G09RevB.01\\State=1-A\\MP2/GTbas1=-689.5108675\\MP4/GTbas1=-689.5976628\\CCSD(T)/G3Bas1=-689.5945752\\MP2/GTbas2=-689.5195185\\MP4/GTbas2=-689.6066935\\MP2/GTbas3=-689.7173936\\MP4/GTbas3=-689.818554\\HF/GTLargeXP=-688.7432228\\MP2/GTLargeXP=-690.4139873\\HF/GFHFB1=-688.7711273\\HF/GFHFB2=-688.775574\\G4=-690.590061\\FreqCoord=-5.4020136362,5.6905859884,-0.431197147,-7.6254547178,4.297138675,-0.105445297,-3.106564036,4.5136705827,-1.2257346746,-3.7220409045,2.1049891926,-1.4899797141,-7.6889922161,1.6906975974,-0.5458095498,-5.4906647411,0.3439132056,-1.3452170725,-5.3267314628,7.7135479092,-0.0960675036,-1.3396679143,5.5014284587,-1.5055505386,-9.4013466315,0.5871098113,-0.3002673767,-5.4376686148,-1.6658961413,-1.710922831,-10.3312069052,5.8166799657,0.854284434\\PG=C01 [X(C6H4Cl1)]\\NImag=0\\

¹m-ethynylphenyl cation

\\1,1\\C,0,-2.9582626013,2.9502879719,-0.3859814777\\C,0,-3.9694427312,2.0213123192,-0.8732320638\\C,0,-1.7748120458,2.4271091225,0.1645339197\\C,0,-1.5498519188,1.0625301929,0.2536309261\\C,0,-3.4832608609,0.8143268308,-0.6592375888\\C,0,-2.4879249094,0.0745031318,-0.1999245608\\H,0,-1.0221151459,3.1156563912,0.5272133615\\H,0,-2.3360259032,-0.9929088012,-0.141502768\\H,0,-0.6338911151,0.6621369538,0.6797910894\\H,0,-4.9050823574,2.3388512035,-1.3096676062\\C,0,-3.2343075702,4.3245689102,-0.4990735513\\C,0,-3.4779406327,5.5009736005,-0.5993544697\\H,0,-3.678632208,6.5451421728,-0.6812252105\\Version=EM64L-G09RevB.01\\State=1-A\\MP2/GTbas1=-306.4117088\\MP4/GTbas1=-306.5058688\\CCSD(T)/G3Bas1=-306.5006575\\MP2/GTbas2=-306.4221672\\MP4/GTbas2=-306.5165187\\MP2/GTbas3=-306.6171559\\MP4/GTbas3=-306.7199428\\HF/GTLargeXP=-305.5177565\\MP2/GTLargeXP=-307.0704437\\HF/GFHFB1=-305.5420313\\HF/GFHFB2=-305.5462064\\G4=-307.230634\\FreqCoord=-5.5903061456,5.5752362801,-0.7293992851,-7.5011596622,3.8197267124,-1.650169451,-3.3539087038,4.5865715362,0.3109240478,-2.9287956731,2.0078910724,0.4792929892,-6.5824090766,1.5388546929,-1.2457784993,-4.7014967179,0.1407905151,-0.3778026672,-1.931517702,5.8877373035,0.9962888669,-4.4144491964,-1.8763257092,-0.2674014785,-1.1978806057,1.2512575052,1.2846189865,-9.2692623148,4.4197882403,-2.4749131008,-6.1119555372,8.1722508831,-0.9431123322,-6.5723553021,10.3953335692,-1.1326158042,-6.9516074167,12.3685262074,-1.2873290826\\PG=C01 [X(C8H5)]\\NImag=0

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¹o-ethynylphenyl cation

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1,1\C,0,-2.7416361302,2.800664121,-0.2615220457\C,0,-3.7063729273,1.8812572808,-0.1931276284\C,0,-1.5635803327,1.9396434943,-0.2357010444\C,0,-1.6104732208,0.5580743571,-0.1576114126\C,0,-4.0514009958,0.6062427624,-0.1160824621\C,0,-2.8244059447,-0.123850166,-0.0970450146\H,0,-0.6329243313,2.4992497809,-0.2842271793\H,0,-5.0351366834,0.1578633494,-0.0733538131\H,0,-2.8991843388,-1.2047099133,-0.0352617124\H,0,-0.6805300829,0.001919341,-0.1436878064\C,0,-2.7120318623,4.1961245865,-0.3401461552\C,0,-2.66035861,5.3953352516,-0.4081485215\H,0,-2.6215845398,6.4595457542,-0.4687452042\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBa s1=-306.4069782\MP4/GTBa s1=-306.5010835\CCSD(T)/G3Ba s1=-306.4962393\MP 2/GTBa s2=-306.4174107\MP4/GTBa s2=-306.511714\MP2/GTBa s3=-306.613306\MP 4/GTBa s3=-306.7160481\HF/GTLa rgeXP=-305.5154254\MP2/GTLa rgeXP=-307.0661517\HF/GFHFB1=-305.5397519\HF/GFHFB2=-305.5439437\G4=-307.2262415\Fre qCoord=-5.1809414421,5.2924881789,-0.494205044,-7.004029779,3.5550610462,-0.3649583263,-2.9547386156,3.6653949997,-0.4454104231,-3.0433533317,1.0546076967,-0.2978424053,-7.6560383366,1.1456327909,-0.2193640622,-5.3373537236,-0.2340428952,-0.1833885002,-1.196053649,4.7228976236,-0.5371115285,-9.5150293733,0.2983184968,-0.1386186176,-5.4786644091,-2.2765718057,-0.0666349795,-1.2860154818,0.0036270289,-0.2715306027,-5.1249974835,7.929526288,-0.6427830785,-5.0273491881,10.1957060206,-0.7712889272,-4.9540768143,12.2067724182,-0.885800062\PG=C01 [X(C8H5)]\NIma g=0\\

¹p-ethynylphenyl cation

\\

1,1\C,0,-2.9659475102,3.0498136165,-0.2109999581\C,0,-4.1527213784,2.3100603432,-0.0524273345\C,0,-1.734038784,2.4427071377,-0.599268975\C,0,-2.0407606176,1.163187434,-0.7351411705\C,0,-4.1442417509,0.9212386262,-0.2802510086\C,0,-2.9649781644,0.2190021559,-0.6715857586\H,0,-2.937472643,4.122239202,-0.0432426678\H,0,-0.8034122433,2.976491026,-0.7311954744\H,0,-5.0418077189,0.3207541814,-0.1669238006\H,0,-2.918891269,-0.845165297,-0.8554891971\C,0,-5.3514320678,2.9610632301,0.3351552765\C,0,-6.3679737098,3.5131595106,0.6638212042\H,0,-7.2687021427,4.0024088333,0.9550288644\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBa s1=-306.4088425\MP4/GTBa s1=-306.5026481\CCSD(T)/G3Ba s1=-306.4980903\MP2/GTBa s2=-306.4194836\MP4/GTBa s2=-306.5134858\MP2/GTBa s3=-306.6144282\MP4/GTBa s3=-306.7168497\HF/GTLa rgeXP=-305.5180231\MP2/GTLa rgeXP=-307.0681335\HF/GFHFB1=-305.5422388\HF/GFHFB2=-305.546418\G4=-307.2287844\Fre qCoord=-5.6048285187,5.7633124915,-0.3987321349,-7.8475061114,4.3653813992,-0.0990733041,-3.2768584055,4.6160475131,-1.1324542427,-3.85647867,2.1981056915,-1.3892154812,-7.8314819377,1.7408887065,-0.5295976547,-5.6029967207,0.4138540972,-1.2691131585,-5.5510188182,7.7899031461,-0.0817167995,-1.5182291117,5.6247528762,-1.3817591961,-9.5276358035,0.6061375589,-0.3154402681,-5.5159051101,-1.5971309484,-1.6166402921,-10.1127410268,5.595598567,0.6333516845,-12.033726333,6.6389093362,1.2544402772,-13.7358563912,7.5634565668,1.8047430027\PG=C01 [X(C8H5)]\NImag=0\\

¹m-(dimethylamino)phenyl cation

\\

1,1\C,0,-2.8994782992,2.6687675851,-0.4092869285\C,0,-3.7901938369,1.673530085,-1.0447740059\C,0,-1.7242175322,2.1629172925,0.2480792023\C,0,-1.4854274078,0.8214757084,0.3941592438\C,0,-3.4114462556,0.4624770772,-0.6943855036\C,0,-2.4926031381,-0.1584888788,0.0228101048\H,0,-1.0395223285,2.865695004,0.7044802528\H,0,-2.5717379172,-1.1092108824,0

.534333662\H,0,-0.6504322936,0.4786379574,0.9974773276\N,0,-3.08470303
59,3.9583445864,-0.6788167675\C,0,-1.9909586934,4.9384169487,-0.694512
7936\C,0,-4.3967574051,4.4715682194,-1.0742856747\H,0,-1.9762257625,5.
5043347289,0.2430954858\H,0,-2.157485781,5.6344446537,-1.5196970835\H,
0,-1.032981034,4.4437673474,-0.8444119776\H,0,-5.1884474474,3.84488315
79,-0.664844124\H,0,-4.4828274316,4.5177644501,-2.167134503\H,0,-4.507
2647205,5.4834505674,-0.6786287024\H,0,-4.3378196796,1.9468543917,-1.9
380872148\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-364.0420206\
MP4/GTBas1=-364.162643\CCSD(T)/G3Bas1=-364.1615374\MP2/GTBas2=-364.056
4041\MP4/GTBas2=-364.1777879\MP2/GTBas3=-364.3176889\MP4/GTBas3=-364.4
51961\HF/GTLargeXP=-362.9727039\MP2/GTLargeXP=-364.849918\HF/GFHFB1=-3
63.0011483\HF/GFHFB2=-363.0065094\G4=-365.0214722\FreqCoord=-5.4792199
137,5.0432398481,-0.7734402047,-7.1624283422,3.1625135359,-1.974336741
8,-3.2582989294,4.0873213309,0.4688017515,-2.8070509909,1.5523641137,0
.7448530236,-6.4466991401,0.8739550186,-1.3121984324,-4.710337289,-0.2
995005761,0.0431048511,-1.9644125099,5.4153787379,1.3312747438,-4.8598
803491,-2.0961047914,1.0097442848,-1.229138903,0.9044946563,1.88495897
3,-5.8292439391,7.4801872079,-1.282777785,-3.7623666724,9.3322555631,-
1.3124389757,-8.3086673683,8.4500393193,-2.0301057136,-3.7345254679,10
.4016851813,0.4593838922,-4.0770572617,10.6475573065,-2.8718112928,-1.
9520512547,8.3975032848,-1.595707381,-9.8047447305,7.2657761815,-1.256
3733153,-8.4713161468,8.5373375435,-4.0952907038,-8.5174959301,10.3622
198357,-1.2824223935,-8.1972912083,3.6790216209,-3.6624540575\PG=C01 [X
(C8H10N1)]\NImag=0\\

¹o-(dimethylamino)phenyl cation

\\1,1\C,0,-2.8300148145,2.7470645054,-0.2988074419\C,0,-3.8191920653,
1.7708058876,-0.4639157749\C,0,-1.614260926,2.1911433055,0.2286722643\
C,0,-1.5332464949,0.828115979,0.3914443585\C,0,-3.7623703594,0.4397317
675,-0.6158367432\C,0,-2.5846434739,-0.0333614433,0.0252744772\H,0,-0.
7328564377,2.8190554576,0.2948420402\H,0,-4.5929672998,-0.2205157759,-
0.8357218728\H,0,-2.5931205212,-1.0641267436,0.3697507507\H,0,-0.61585
16502,0.3893458385,0.768609594\N,0,-3.0212013855,4.0126406719,-0.68149
5924\C,0,-2.0602513933,5.0786613821,-0.4234985557\C,0,-4.1848556791,4.
2672743587,-1.5104519012\H,0,-1.5777582042,4.9257022662,0.5425182797\H
,0,-2.6024479059,6.025999626,-0.4009514683\H,0,-1.3014915417,5.1336247
205,-1.2126385172\H,0,-4.9603794774,3.5385408222,-1.1889318105\H,0,-3.
9932822869,4.0841311766,-2.5726454612\H,0,-4.5350080832,5.2903961975,-
1.3700062937\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-364.02539
53\MP4/GTBas1=-364.1468368\CCSD(T)/G3Bas1=-364.148816\MP2/GTBas2=-364.
0396879\MP4/GTBas2=-364.1619686\MP2/GTBas3=-364.3006478\MP4/GTBas3=-36
4.436014\HF/GTLargeXP=-362.9614244\MP2/GTLargeXP=-364.8323427\HF/GFHFB
1=-362.9900201\HF/GFHFB2=-362.9953928\G4=-365.0089503\FreqCoord=-5.347
9529515,5.1911995846,-0.5646642316,-7.2172270523,3.3463381621,-0.87667
37633,-3.0505110572,4.1406607653,0.4321279537,-2.8974159695,1.56491240
65,0.7397226339,-7.1098495897,0.8309726124,-1.1637627872,-4.8842683168
, -0.0630439912,0.0477618401,-1.3848979619,5.3272427684,0.5571707084,-8
.679450334,-0.4167144244,-1.5792854628,-4.9002876147,-2.0109081161,0.6
987276562,-1.1637909573,0.7357570058,1.4524616357,-5.7092432109,7.5827
919396,-1.287840657,-3.8933108983,9.5972791339,-0.8002962879,-7.908231
1391,8.0639798718,-2.8543404303,-2.9815309098,9.3082282952,1.025210970
7,-4.9179138173,11.38748897,-0.7576884676,-2.4594625781,9.7011447907,-
2.2915546958,-9.3737587275,6.6868730639,-2.2467555126,-7.5462098935,7.
7178894146,-4.8615953587,-8.5699232876,9.9973999477,-2.5889366955\PG=C
01 [X(C8H10N1)]\NImag=0\\

¹p-(dimethylamino)phenyl cation

```
\1,1\C,0,-2.8732964189,3.0064728231,-0.1647277133\C,0,-4.0996377295,
2.269720566,-0.0604118841\C,0,-1.6681653498,2.3637731536,-0.4419628641
\C,0,-1.9167038964,1.0932054693,-0.8527365034\C,0,-4.0627887564,0.8467
544752,-0.2387322414\C,0,-2.8680932978,0.1844391279,-0.5160556703\H,0,
-2.8619450577,4.0862345412,-0.0955279314\H,0,-0.720260955,2.8847415878
,-0.4955449221\H,0,-4.9713932516,0.2591557701,-0.230462431\H,0,-2.8013
129271,-0.8908073449,-0.6261436184\N,0,-5.2578868875,2.8976292796,0.21
968471111\C,0,-5.2902949672,4.3399186959,0.4759133995\C,0,-6.4980365835
,2.140407538,0.4087135765\H,0,-6.6832604993,1.4870342925,-0.4497378998
\H,0,-7.3287349813,2.8383797657,0.4880750184\H,0,-6.4624863478,1.53430
94199,1.3200067996\H,0,-4.8047290703,4.8851636787,-0.3394191731\H,0,-4
.7954983282,4.5906566834,1.4201247772\H,0,-6.3270946948,4.6651404769,0
.5298645702\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-364.017545
\MP4/GTBas1=-364.139834\CCSD(T)/G3Bas1=-364.1418454\MP2/GTBas2=-364.03
16978\MP4/GTBas2=-364.1548416\MP2/GTBas3=-364.2929768\MP4/GTBas3=-364.
4293077\HF/GTLargeXP=-362.9621176\MP2/GTLargeXP=-364.8253852\HF/GFHFB1
=-362.9907014\HF/GFHFB2=-362.9960821\G4=-365.0028974\FreqCoord=-5.4297
433303,5.6814102617,-0.3112902647,-7.7471925528,4.2891502679,-0.114161
9162,-3.1523756554,4.4668839006,-0.8351887741,-3.622045442,2.065858944
,-1.6114384549,-7.6775580854,1.60013406,-0.4511385553,-5.4199108565,0.
3485394399,-0.9752038862,-5.4082923665,7.7218641976,-0.1805216283,-1.3
610959491,5.4513715652,-0.9364441893,-9.3945717444,0.4897334312,-0.435
5108785,-5.2937142447,-1.6833819191,-1.1832399587,-9.935966255,5.47572
57731,0.4151439395,-9.9972086501,8.2012577742,0.899345988,-12.27950954
43,4.0447840596,0.7723567263,-12.6295320185,2.8100875629,-0.8498814622
,-13.8493020152,5.3637604184,0.922328117,-12.2123293348,2.8994246067,2
.4944513448,-9.0796220855,9.2316214672,-0.6414092814,-9.0621785111,8.6
750839017,2.6836469035,-11.9564761901,8.8158378728,1.0012989252\PG=C01
[X(C8H10N1)]\NImag=0\\
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¹syn-m-thiomethoxyphenyl cation

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\
\1,1\C,0,-0.2703178765,1.2136560608,-0.1210086609\C,0,-1.588861379,1.2
557567248,-0.1043311574\C,0,-2.6882012185,0.5328315004,0.0393143575\C,
0,-2.26519144,-0.8445560275,0.0404742744\C,0,-0.925199557,-1.170986931
8,0.101029552\C,0,0.0957797321,-0.1886339927,0.0417081524\H,0,0.424642
9814,1.9553717935,-0.4889568963\H,0,-3.6769681248,0.8471980045,0.34642
35964\H,0,-3.0345795723,-1.5993295066,0.1728722733\H,0,-0.637313178,-2
.210090229,0.2108836937\S,0,1.7283664688,-0.7073783442,-0.1817823457\C
,0,2.7235949245,0.7435116882,0.2659764542\H,0,2.422483414,1.1369080333
,1.2372681763\H,0,3.7497020853,0.3736027096,0.3185238678\H,0,2.6715067
4,1.5083715169,-0.5131473378\\Version=EM64L-G09RevB.01\State=1-A\MP2/G
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\MP2/GTBas2=-667.3127235\MP4/GTBas2=-667.421279\MP2/GTBas3=-667.547661
4\MP4/GTBas3=-667.6702294\HF/GTLargeXP=-666.4128323\MP2/GTLargeXP=-668
.2928946\HF/GFHFB1=-666.4411729\HF/GFHFB2=-666.4468793\G4=-668.4761935
\FreqCoord=-0.5108267555,2.2934775744,-0.2286732289,-3.0025128695,2.37
30362993,-0.1971573146,-5.079964093,1.0069056107,0.0742933688,-4.28059
14602,-1.5959795959,0.076485294,-1.748373781,-2.2128446063,0.190918184
7,0.1809974627,-0.3564665855,0.0788169856,0.8024589391,3.6951171777,-0
.9239946248,-6.9484627553,1.6009722089,0.6546457231,-5.7345243201,-3.0
222947637,0.3266812525,-1.2043473672,-4.1764652618,0.398512427,3.26613
92832,-1.3367513429,-0.3435188492,5.1468485042,1.4050334673,0.50262265
62,4.577830214,2.1484448212,2.3380980062,7.0859100212,0.7060068036,0.6
01922877,5.0484161007,2.8504090736,-0.9697079343\PG=C01 [X(C7H7S1)]\NI
mag=0\\
```

¹syn-o-thiomethoxyphenyl cation

\

\1,1\C,0,-0.5046643696,0.8702498652,-0.1190069907\C,0,-1.6913450434,1.4577284423,-0.0203677981\C,0,-2.635205575,0.3928844641,0.0722090241\C,0,-2.1928697702,-0.932060011,0.0820186809\C,0,-0.8481636323,-1.2503737376,0.0052842893\C,0,0.2059303427,-0.2516850762,-0.0979212354\H,0,-1.960203219,2.4980556142,-0.1434359115\H,0,-3.6851709998,0.6654186011,0.0461059954\H,0,-2.91521536,-1.7355025068,0.1667183277\H,0,-0.4866197916,-2.270221675,0.1203428656\S,0,1.8936285689,-0.6545618333,-0.0639806631\C,0,2.6657997891,0.9870049051,0.134359282\H,0,2.4304522603,1.4134592967,1.1095708741\H,0,3.7385493712,0.7943510389,0.0735309583\H,0,2.3742004288,1.6496466122,-0.6833936985\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTbas1=-667.2949862\MP4/GTbas1=-667.4019072\CCSD(T)/G3bas1=-667.3993963\MP2/GTbas2=-667.3056605\MP4/GTbas2=-667.4132308\MP2/GTbas3=-667.5415125\MP4/GTbas3=-667.6633458\HF/GTLargeXP=-666.4160458\MP2/GTLargeXP=-668.2860699\HF/GFHFB1=-666.4445465\HF/GFHFB2=-666.4502545\G4=-668.4688385\FreqCoord=-0.9536774475,1.6445339124,-0.2248906202,-3.1961789283,2.7547075321,-0.0384895604,-4.9798168406,0.742444039,0.1364552798,-4.1439233107,-1.7613381602,0.1549928446,-1.6027969809,-2.3628639278,0.0099858597,0.3891519501,-0.4756158658,-0.1850443175,-3.7042472488,4.7206409756,-0.2710545903,-6.9639639425,1.2574589198,0.0871277044,-5.5089586488,-3.2796244407,0.3150519807,-0.919578137,-4.2900972266,0.227415058,3.5784393926,-1.236942602,-0.1209059311,5.0376315265,1.8651689624,0.2539022464,4.592889151,2.6710509708,2.096785077,7.0648344459,1.501105917,0.1389533735,4.4865885949,3.1173803131,-1.2914269312\PG=C01 [X(C7H7S1)]\NImag=0\\

¹p-thiomethoxyphenyl cation

\

\1,1\C,0,-0.3711715618,1.1395112024,-0.0410352098\C,0,-1.7405088924,1.4890885348,0.0339874933\C,0,-2.4346532005,0.3539088207,-0.0999249607\C,0,-2.3040246981,-0.963949966,0.1064065468\C,0,-0.9225901585,-1.2418942369,0.0500203902\C,0,0.0428504933,-0.2083965404,-0.0194615179\H,0,0.3324586054,1.9552904337,-0.1587485046\H,0,-2.1026898432,2.5081078771,0.0713923168\H,0,-3.0684213897,-1.7276954563,0.1612441145\H,0,-0.628728873,-2.2875336534,0.0111784656\S,0,1.7012499227,-0.7373802348,-0.0802612369\C,0,2.6722514067,0.7849323116,0.1070845428\H,0,2.4677621316,1.2671408078,1.0637661267\H,0,3.7121362376,0.4541424852,0.0845674335\H,0,2.4996858199,1.4645516144,-0.7309150004\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTbas1=-667.2894464\MP4/GTbas1=-667.3973245\CCSD(T)/G3bas1=-667.396535\MP2/GTbas2=-667.3003124\MP4/GTbas2=-667.4088182\MP2/GTbas3=-667.5353596\MP4/GTbas3=-667.6580711\HF/GTLargeXP=-666.4092114\MP2/GTLargeXP=-668.2802956\HF/GFHFB1=-666.4376902\HF/GFHFB2=-666.4433646\G4=-668.4653374\FreqCoord=-0.7014126002,2.153364098,-0.0775453084,-3.2890851386,2.8139695183,0.0642270544,-4.6008277775,0.6687907472,-0.1888308096,-4.3539756828,-1.8216014416,0.2010792322,-1.7434427325,-2.3468399938,0.0945248386,0.0809756971,-0.3938123884,-0.036776939,0.6282557148,3.69496343,-0.2999911977,-3.9735079461,4.7396369995,0.1349119268,-5.7984760869,-3.2648712535,0.304707217,-1.1881253818,-4.3228121246,0.0211242385,3.2148964375,-1.3934466996,-0.1516717569,5.0498233169,1.4833071018,0.202360459,4.6633945898,2.3945490986,2.0102266489,7.0149208571,0.8582049224,0.159809289,4.7237216179,2.7676014587,-1.3812291772\PG=C01 [X(C7H7S1)]\NImag=0\\

¹syn-m-methoxyphenyl cation

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\1,1\C,0,1.2388739653,-1.2117427224,-0.0186943332\C,0,-0.0802180973,-1

```
.1532263875,-0.0491054784\C,0,-0.4409603319,0.2550351087,0.0141059292\
C,0,0.595700528,1.2227442485,-0.0078035276\C,0,1.9197408959,0.85218221
26,-0.0238216376\C,0,2.3628214662,-0.5317958561,0.0405718955\H,0,-0.77
3610901,-1.9032537786,-0.4076041595\H,0,0.3153639999,2.2684292668,0.01
02839579\H,0,2.706069896,1.592573585,0.0977744835\H,0,3.356947686,-0.8
184835805,0.3514997502\O,0,-1.6794094484,0.6568228058,-0.1123334112\C,
0,-2.7811768272,-0.2445333921,0.1218362959\H,0,-2.624652815,-0.8029074
681,1.0481653976\H,0,-3.6607699515,0.3916819795,0.2015736355\H,0,-2.89
34090649,-0.9191500217,-0.7328717977\\Version=EM64L-G09RevB.01\State=1
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49,-2.1792820416,-0.0927959058,-0.8332942627,0.4819465097,0.026656343,
1.1257108551,2.3106517603,-0.01474653,3.6277845394,1.6103909971,-0.045
016371,4.465085472,-1.0049485267,0.0766697711,-1.4619127364,-3.5966284
029,-0.770260232,0.595951592,4.286710066,0.0194338639,5.1137309998,3.0
095279222,0.1847669966,6.3437117689,-1.5467098114,0.6642382636,-3.1736
239225,1.2412152208,-0.2122793827,-5.2556625306,-0.4621011414,0.230237
2323,-4.9598750143,-1.5172752247,1.9807455434,-6.9178526438,0.74017167
24,0.3809189666,-5.467750723,-1.7369418161,-1.3849269882\PG=C01 [X(C7H
7O1)]\NImag=0\\
```

¹syn-o-methoxyphenyl cation

```
\
\1,1\C,0,-1.3496507949,1.4112771453,0.0158660867\C,0,-0.1333641303,0.8
842959891,-0.0588592095\C,0,0.5700651976,-0.261467636,-0.1445408891\C,
0,-0.4845836408,-1.2462334032,-0.0368105578\C,0,-1.8382120363,-0.95902
01907,0.0576979656\C,0,-2.3029498504,0.3527041968,0.1062281906\H,0,-1.
6303088888,2.4380330795,-0.1897675663\H,0,-0.0847238165,-2.2407260603,
0.1628763873\H,0,-2.5397257154,-1.7828125018,0.1247611747\H,0,-3.35415
98742,0.6153535667,0.0640920245\O,0,1.829624787,-0.5904390136,-0.13653
22415\C,0,2.7808143738,0.4641899067,0.1642861894\H,0,2.7162811628,0.72
66444326,1.2225469017\H,0,3.7596273275,0.051896703,-0.0698169636\H,0,2
.5695178991,1.332750786,-0.4711854926\\Version=EM64L-G09RevB.01\State=
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.9235212\MP4/GTbas3=-345.0352156\HF/GTLargeXP=-343.7407901\MP2/GTLarge
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5756294\FreqCoord=-2.5504703774,2.6669273022,0.0299825587,-0.252021682
2,1.6710772397,-0.1112277864,1.0772671014,-0.4941022246,-0.2731426953,
-0.9157303696,-2.3550398296,-0.0695618731,-3.4737173229,-1.8122855164,
0.1090333533,-4.351944515,0.6665143378,0.2007421878,-3.0808373119,4.60
72148232,-0.3586087292,-0.1601048101,-4.2343585929,0.3077917655,-4.799
3860548,-3.3690273746,0.2357644522,-6.3384435681,1.1628497159,0.121116
3735,3.4574897733,-1.1157680339,-0.2580085447,5.2549775929,0.877191797
2,0.3104559054,5.1330274975,1.3731589737,2.3102788287,7.1046660106,0.0
980705559,-0.1319349407,4.8556851229,2.5185339889,-0.8904115387\PG=C01
[X(C7H7O1)]\NImag=0\\
```

¹p-methoxyphenyl cation

```
\
\1,1\C,0,-1.3650727508,1.477017742,0.0474462369\C,0,0.0023365523,1.096
7953804,-0.0029210499\C,0,0.3725947355,-0.2646687954,-0.0026882284\C,0
,-0.6186082131,-1.276741968,0.0098509026\C,0,-1.9980153754,-0.97693464
16,0.047964982\C,0,-2.0577886789,0.3494978304,-0.0752335321\H,0,-1.711
```

5183802,2.4995404082,0.1118198587\H,0,0.7284947457,1.8987062566,-0.057
4542391\H,0,-0.327083474,-2.3196649528,-0.0693582536\H,0,-2.7832589169
, -1.7201409309,0.0428914938\O,0,1.6214371442,-0.7042262328,-0.02718663
8\C,0,2.7114635165,0.2319479282,0.0143098105\H,0,2.6813158901,0.816462
8074,0.9385922333\H,0,3.6145058766,-0.3749125245,-0.010929024\H,0,2.68
36413283,0.8891296927,-0.8612685528\\Version=EM64L-G09RevB.01\State=1-
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,2.0726428927,-0.0055199844,0.7041020086,-0.5001515392,-0.0050800155,-
1.1690001063,-2.4126926618,0.0186155081,-3.7757018688,-1.8461389224,0.
09064068,-3.8886570424,0.6604551834,-0.1421707718,-3.2343010099,4.7234
468296,0.2113089092,1.3766555586,3.5880348318,-0.108572777,-0.61809818
84,-4.3835314808,-0.1310681043,-5.2595971098,-3.2505952694,0.081053176
7,3.0640721443,-1.3307947156,-0.0513753004,5.1239234654,0.4383180615,0
.027041623,5.0669527081,1.5428911037,1.7736822714,6.8304262125,-0.7084
81995,-0.0206528622,5.0713471494,1.6802116158,-1.6275616917\PG=C01 [X(
C7H7O1)]\NImag=0\\

¹anti-o-thiomethoxyphenyl cation

\
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242740382,-0.0004417656\C,0,-2.1961459093,2.9596243628,-0.0019297461\C
,0,-4.7631747504,1.5316445136,-0.0010966216\C,0,-3.5483733264,0.784696
0274,-0.0021315737\C,0,-2.5788397035,1.6882666641,-0.0015031015\H,0,-5
.6908457268,0.9698934717,0.000660632\S,0,-0.6088696546,3.6799300313,-0
.0057279607\H,0,-3.4591316596,4.6917418727,-0.002202989\H,0,-5.6268254
876,3.498071948,0.0000013614\C,0,-0.9850207681,5.4586448015,-0.0031566
873\H,0,0.0019160501,5.9275887237,-0.0043373618\H,0,-1.5152268666,5.75
13035735,0.9040770115\H,0,-1.5182784137,5.7532155829,-0.9079929082\H,0
, -3.486059197,-0.2949748398,-0.0009408187\\Version=EM64L-G09RevB.01\St
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=-667.3992662\MP2/GTBas2=-667.3055411\MP4/GTBas2=-667.4129671\MP2/GTBa
s3=-667.5421081\MP4/GTBas3=-667.6637977\HF/GTLargeXP=-666.4166724\MP2/
GTLargeXP=-668.2866861\HF/GFHFB1=-666.4452291\HF/GFHFB2=-666.4509298\G
4=-668.4691106\FreqCoord=-6.6125673306,6.8151824564,-0.0015447957,-8.8
961213533,5.5260770697,-0.000834816,-4.1501143164,5.5928795019,-0.0036
466916,-9.0010958013,2.8943886636,-0.0020723145,-6.7054538041,1.482860
5893,-0.0040280905,-4.8733007802,3.1903616344,-0.0028404502,-10.754139
8882,1.8328330396,0.0012484136,-1.1505968978,6.9540599473,-0.010824277
, -6.5368114942,8.8661072256,-0.0041630459,-10.6331591691,6.6103979748,
0.0000025727,-1.8614194869,10.3153437315,-0.0059652745,0.0036208099,11
.2015193162,-0.0081964259,-2.8633638071,10.868388661,1.7084579548,-2.8
691303954,10.8720018351,-1.7158579271,-6.5876971654,-0.5574216633,-0.0
017778897\PG=C01 [X(C7H7S1)]\NImag=0\\

¹anti-o-methoxyphenyl cation

\
\1,1\C,0,-1.3301721333,1.4526716129,-0.0716182421\C,0,-0.1744739872,0.
8084934329,-0.0269319118\C,0,0.4633363969,-0.3756641691,0.0575972144\C
,0,-0.6642826828,-1.2730152708,0.1239356493\C,0,-1.994891872,-0.875179
7593,0.0974850261\C,0,-2.3563027158,0.4647835568,0.0013894302\H,0,-1.5
09720158,2.5178097842,-0.145883729\H,0,-0.3845826355,-2.3218055738,0.1
966341949\H,0,-2.7645455331,-1.6358809663,0.153431871\H,0,-3.382754839
4,0.8131495236,-0.020543219\O,0,1.7438278607,-0.6410817483,0.073013499

5\ C,0,2.183547193,-2.0175480432,0.1721677194\ H,0,1.83669469,-2.4581069
879,1.1102850305\ H,0,3.2699337666,-1.9565034815,0.1657493035\ H,0,1.833
49665,-2.5888919102,-0.6912618369\ \Version=EM64L-G09RevB.01\State=1-A\
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921696\MP4/GTBas3=-345.0331923\HF/GTLargeXP=-343.7439568\MP2/GTLargeXP
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2553123453,-2.4056502248,0.2342044353,-3.7697993028,-1.6538500622,0.18
42200013,-4.4527668191,0.8783136333,0.0026256426,-2.8529576359,4.75797
09469,-0.2756802951,-0.7267558566,-4.3875766682,0.3715847767,-5.224233
9394,-3.0913670123,0.2899442162,-6.3924802212,1.5366299047,-0.03882105
78,3.2953570796,-1.2114689331,0.1379755181,4.126306193,-3.8126132617,0
.3253498386,3.4708499538,-4.6451490124,2.098134637,6.1792792915,-3.697
255758,0.3132207902,3.4648065341,-4.8922966979,-1.3062955579\PG=C01 [X
(C7H7O1)]\NImag=1\

¹p-hydroxyphenyl cation

\1,1\ C,0,-2.6811752068,2.4002677697,0.\ C,0,-3.942399206,1.9997214288,
0.\ C,0,-1.4010138634,2.0545011052,0.\ C,0,-1.424832751,0.6349649388,0.\
C,0,-3.8668838879,0.5763811331,0.\ C,0,-2.6310107057,-0.0932483077,0.\ H
,0,-4.8656920729,2.5621246569,0.\ H,0,-0.4993999382,2.6508199059,0.\ H,0
, -0.468384535,0.1210320324,0.\ H,0,-4.8151916248,0.046708576,0.\ O,0,-2.
5113094911,-1.4226968476,0.\ H,0,-3.3652267172,-1.8731163915,0.\ \Versio
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6012047\CCSD(T)/G3Bas1=-305.5979012\MP2/GTBas2=-305.5328747\MP4/GTBas2
=-305.6142322\MP2/GTBas3=-305.7362627\MP4/GTBas3=-305.8269237\HF/GTLar
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/GFHFB2=-304.7423736\G4=-306.313366\FreqCoord=-5.0666868552,4.53584873
02,0.,-7.4500548058,3.7789258424,0.,-2.6475325102,3.8824444286,0.,-2.6
925436846,1.1999098383,0.,-7.3073515357,1.0892024897,0.,-4.9718896864,
-0.1762137639,0.,-9.1948254646,4.8417139199,0.,-0.943729114,5.00932364
98,0.,-0.885118496,0.2287173945,0.,-9.0993934483,0.0882664167,0.,-4.74
56871731,-2.688507412,0.,-6.3593568706,-3.539676995,0.\PG=CS [SG(C6H5O
1)]\NImag=1\

¹p-thiolphenyl cation

\1,1\ C,0,-2.6838883582,2.4606269558,0.\ C,0,-3.9407277426,2.0510547321
,0.\ C,0,-1.404990165,2.1186880834,0.\ C,0,-1.4239211416,0.6932976895,0.
\ C,0,-3.8510057523,0.6246110789,0.\ C,0,-2.6192955458,-0.0481203797,0.\
H,0,-4.8728773476,2.5982454514,0.\ H,0,-0.5027868431,2.7138253121,0.\ H,
0,-0.4481494577,0.2153105773,0.\ H,0,-4.8037491541,0.1044232537,0.\ S,0,
-2.4772330926,-1.8041702168,0.\ H,0,-3.7957253995,-2.0714125376,0.\ \Ver
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as2=-628.2170677\MP2/GTBas3=-628.3277777\MP4/GTBas3=-628.4316546\HF/GT
LargeXP=-627.3621182\MP2/GTLargeXP=-629.0130092\HF/GFHFB1=-627.3876688
\HF/GFHFB2=-627.3926277\G4=-629.1831724\FreqCoord=-5.0718139682,4.6499
110616,0.,-7.4468961979,3.8759317272,0.,-2.6550466313,4.0037402385,0.,
-2.6908209925,1.3101427617,0.,-7.2773462079,1.1803438787,0.,-4.9497512
426,-0.0909343391,0.,-9.208403666,4.9099723291,0.,-0.9501294366,5.1283
866123,0.,-0.8468797416,0.4068780246,0.,-9.0777703123,0.1973313513,0.,
-4.6812921124,-3.4093876069,0.,-7.1728814807,-3.9144024042,0.\PG=CS [S
G(C6H5S1)]\NImag=1\

¹m-nitrophenyl cation

```
\1,1\ C,0,-2.7610183094,2.8721114291,0.\ C,0,-3.9537348772,2.16402502
76,0.\ C,0,-1.4726979751,2.2665465906,0.\ C,0,-1.7589377474,0.979971661,
0.\ C,0,-3.9293398255,0.7688373368,0.\ C,0,-2.7000500088,0.042610576,0.\
N,0,-2.7413169376,4.3902235742,0.\ H,0,-4.8907770687,2.7057033928,0.\ H,
0,-4.8408873514,0.1772551258,0.\ H,0,-2.6214398229,-1.0365747911,0.\ H,0
,-0.5611400738,2.8550350268,0.\ O,0,-1.6529685137,4.9196598233,0.\ O,0,-
3.8382314886,4.9029152272,0.\ \Version=EM64L-G09RevB.01\State=1-A'\MP2/
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\MP2/GTBas2=-434.4930856\MP4/GTBas2=-434.5912709\MP2/GTBas3=-434.75607
32\MP4/GTBas3=-434.8676999\HF/GTLargeXP=-433.3370079\MP2/GTLargeXP=-43
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\FreqCoord=-5.2175684527,5.4275040242,0.,-7.4714761199,4.0894146469,0.
,-2.7829958494,4.2831523236,0.,-3.3239106274,1.8518780573,0.,-7.425376
1532,1.4528920073,0.,-5.1023550617,0.0805223189,0.,-5.1803382554,8.296
3202173,0.,-9.2422292369,5.1130384091,0.,-9.1479513344,0.3349636434,0.
,-4.9538033392,-1.9588424715,0.,-1.0604010616,5.3952343004,0.,-3.12365
77971,9.2968097329,0.,-7.253206348,9.2651670323,0.\PG=CS [SG(C6H4N1O2)
]\NImag=0\
```

¹o-nitrophenyl cation

```
\1,1\ C,0,-3.1648799594,3.2243110685,0.\ C,0,-4.0703364861,2.22641418
97,0.\ C,0,-1.7721747212,2.8850893482,0.\ C,0,-1.2424862074,1.2178612568
,0.\ C,0,-3.6831299781,0.8311304955,0.\ C,0,-2.4096701786,0.3729143525,0
.\ H,0,-3.4325242091,4.2742500068,0.\ H,0,-5.1274449832,2.463681471,0.\ N
,0,-0.7089257566,3.5097114719,0.\ H,0,-4.4808941823,0.0948175065,0.\ H,0
,-2.1715362512,-0.6864029241,0.\ O,0,-0.0809217074,1.0269407465,0.\ O,0,
0.4451446207,3.6002310102,0.\ \Version=EM64L-G09RevB.01\State=1-A'\MP2/
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4\MP2/GTBas2=-434.5700765\MP4/GTBas2=-434.674822\MP2/GTBas3=-434.83525
95\MP4/GTBas3=-434.9533967\HF/GTLargeXP=-433.4056884\MP2/GTLargeXP=-43
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\FreqCoord=-5.9807563667,6.0930648866,0.,-7.6918212274,4.2073130769,0.
,-3.3489248826,5.452028737,0.,-2.3479586559,2.3014242432,0.,-6.9601069
704,1.5706090171,0.,-4.553616708,0.7047059972,0.,-6.4865306997,8.07716
19363,0.,-9.6894667798,4.6556832589,0.,-1.3396755286,6.6323934873,0.,-
8.4676628351,0.17917912,0.,-4.1036088025,-1.2971135434,0.,-0.152919865
1,1.9406367657,0.,0.8412014226,6.8034506243,0.\PG=CS [SG(C6H4N1O2)]\NI
mag=0\
```

¹p-nitrophenyl cation

```
\1,1\ C,0,-2.7003694602,2.8889393311,0.\ C,0,-3.8638823653,2.12544737
93,0.\ C,0,-1.4231787822,2.254165628,0.\ C,0,-1.7256186434,0.9643184346,
0.\ C,0,-3.8706514235,0.7338169447,0.\ C,0,-2.6427540922,0.0082658428,0.
\N,0,-5.1712177749,2.8353611484,0.\ O,0,-5.1198357809,4.0505525674,0.\ O
,0,-6.1624528359,2.1305322168,0.\ H,0,-2.7408791092,3.974894145,0.\ H,0,
-0.4711566335,2.7685743844,0.\ H,0,-4.8035313994,0.1764354654,0.\ H,0,-2
.5557816993,-1.0703434878,0.\ \Version=EM64L-G09RevB.01\State=1-A'\MP2/
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778\MP4/GTBas3=-434.8666054\HF/GTLargeXP=-433.3395782\MP2/GTLargeXP=-4
35.3325086\HF/GFHFB1=-433.3751376\HF/GFHFB2=-433.3818702\G4=-435.54180
85\FreqCoord=-5.1029587375,5.4593041503,0.,-7.3016794801,4.0165134566,
0.,-2.6894181365,4.259755695,0.,-3.2609466458,1.8222977462,0.,-7.31447
11463,1.3867130572,0.,-4.9940814708,0.0156201792,0.,-9.7721853681,5.35
80560582,0.,-9.6750874713,7.6544350393,0.,-11.6453481666,4.0261224071,
0.,-5.1795108798,7.5114613412,0.,-0.890357003,5.231847365,0.,-9.077358
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8157,0.3334147097,0.,-4.8297274671,-2.02265606,0.\PG=CS [SG(C6H4N1O2)]
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³m-aminophenyl cation

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2.0381000612,-0.8766120765\C,0,-1.778051988,2.5006413444,0.1567844014\
C,0,-1.5311133054,1.1538209682,0.2563621245\C,0,-3.6731794654,0.735685
0652,-0.7400855505\C,0,-2.4953373767,0.2202259151,-0.2004562794\H,0,-1
.0486464364,3.2253105612,0.5028522465\H,0,-2.3163766234,-0.8474498195,
-0.1295748674\H,0,-0.600380599,0.7982162402,0.683755199\H,0,-4.9345415
367,2.3830595201,-1.305512685\N,0,-3.2345800205,4.2873621097,-0.499858
6823\H,0,-4.0921926654,4.6541321671,-0.8939409571\H,0,-2.5539601015,4.
9647505652,-0.178417459\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1
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GTBas2=-285.6989484\MP4/GTBas2=-285.7926621\MP2/GTBas3=-285.8863124\MP
4/GTBas3=-285.9902904\HF/GTLargeXP=-284.9383895\MP2/GTLargeXP=-286.299
0331\HF/GFHFB1=-284.9612684\HF/GFHFB2=-284.9654653\G4=-286.4581553\Fre
qCoord=-5.6928046259,5.6266506825,-0.7747979457,-7.5571233146,3.851450
9472,-1.6565567493,-3.3600313073,4.7255272975,0.2962795805,-2.89338482
56,2.1804056363,0.4844542062,-6.9413032266,1.3902432932,-1.3985590054,
-4.7155042511,0.4161666669,-0.3788074697,-1.981654575,6.0949536542,0.9
502530311,-4.3773174389,-1.6014480703,-0.244861013,-1.1345549076,1.508
4100889,1.292110068,-9.3249320958,4.5033298513,-2.4670614377,-6.112470
3937,8.1019402198,-0.9445960147,-7.7331234206,8.795035182,-1.689303587
8,-4.8262851461,9.3820188864,-0.3371601349\PG=C01 [X(C6H6N1)]\NImag=0\
\

³o-aminophenyl cation

\\1,3\C,0,-2.7297030942,2.6886066899,-0.1823857369\C,0,-3.9459441385
,1.9590023773,-0.1391233144\C,0,-1.5126247413,1.9214679656,-0.19560416
26\C,0,-1.5879346467,0.5545075316,-0.1666186993\C,0,-4.0547107831,0.60
90871923,-0.1100449167\C,0,-2.8392904334,-0.1155629924,-0.1241181729\H
,0,-0.5590700568,2.4390460092,-0.2277133589\H,0,-5.0104834216,0.097849
2582,-0.0772779806\H,0,-2.8657850535,-1.2001336173,-0.102254293\H,0,-0
.6778227465,-0.033930773,-0.1759598731\N,0,-2.724411636,4.0173282883,-
0.2101100112\H,0,-3.591087753,4.5417138694,-0.2008273767\H,0,-1.860101
4954,4.5439482008,-0.2418221038\\Version=EM64L-G09RevB.01\State=3-A\MP
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7019779868,-0.2629049628,-2.8584465028,3.631048228,-0.3696382978,-3.00
07615992,1.0478673734,-0.3148637102,-7.6622929282,1.1510079845,-0.2079
547549,-5.3654813309,-0.2183824067,-0.234549355,-1.0564892965,4.609128
9828,-0.4303158851,-9.4684414602,0.1849083003,-0.1460342194,-5.4155489
068,-2.2679238595,-0.1932326096,-1.2808993575,-0.0641198684,-0.3325159
705,-5.1483918653,7.5916502508,-0.3970503789,-6.7861723722,8.582595387
2,-0.379508742,-3.5150824057,8.5868176615,-0.456977549\PG=C01 [X(C6H6N
1)]\NImag=0\\

³p-aminophenyl cation

\\1,3\C,0,-2.8831529335,3.0594277661,-0.2626257181\C,0,-4.0996385674
,2.3057963082,-0.1280881455\C,0,-1.7174817115,2.4076889786,-0.59166435
78\C,0,-1.8046806035,1.0288215671,-0.7747655093\C,0,-4.1138364693,0.88
31953767,-0.3327867381\C,0,-2.9454704986,0.2362220572,-0.6616732067\H,
0,-2.9023956185,4.1328713203,-0.1023353161\H,0,-0.7808431022,2.9426088

196,-0.7014752974\H,0,-5.0473627779,0.3398974535,-0.2246187929\H,0,-2.9174049966,-0.8354983973,-0.8232810525\N,0,-5.229794993,2.9346138077,0.1913702103\H,0,-5.2557211328,3.9351643481,0.343485494\H,0,-6.1041265952,2.4349205942,0.2951184303\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-285.685837\MP4/GTBas1=-285.780324\CCSD(T)/G3Bas1=-285.7969015\MP2/GTBas2=-285.6959956\MP4/GTBas2=-285.7910552\MP2/GTBas3=-285.8829698\MP4/GTBas3=-285.9884455\HF/GTLargeXP=-284.9544215\MP2/GTLargeXP=-286.2950469\HF/GFHFB1=-284.9773335\HF/GFHFB2=-284.9815357\G4=-286.4615998\FreqCoord=-5.4483694435,5.7814806012,-0.4962906827,-7.7471941361,4.3573235408,-0.2420515159,-3.2455700729,4.5498727827,-1.1180835989,-3.410352098,1.9441910014,-1.4640946299,-7.7740242824,1.6689973838,-0.6288757957,-5.5661325749,0.4463949947,-1.2503811501,-5.4847328483,7.8099949378,-0.1933857212,-1.4755796159,5.5607247853,-1.3255962011,-9.5381333436,0.6423131003,-0.4244680029,-5.5130964622,-1.5788631554,-1.5557757196,-9.882880268,5.5456164024,0.3616372875,-9.9318735719,7.4363829058,0.6490935143,-11.5351275453,4.6013330784,0.55769301\PG=C01 [X(C6H6N1)]\NImag=0\\

³m-cyanophenyl cation

\1,3\C,0,-3.0025665104,3.0909873368,-0.5330527741\C,0,-4.0070352201,2.1863629301,-0.9764919231\C,0,-1.7734867085,2.6047231777,0.0753957079\C,0,-1.5539647422,1.2552050407,0.2362582688\C,0,-3.7144941412,0.8770191857,-0.7823363401\C,0,-2.5414968014,0.3479116486,-0.1989637387\H,0,-1.0391644336,3.3353894691,0.3967088511\H,0,-2.4076189636,-0.7249221182,-0.0905343776\H,0,-0.6390952501,0.8909155009,0.6892553171\H,0,-4.9243426715,2.5443585234,-1.4303958795\C,0,-3.1761407207,4.4764304663,-0.6734063838\N,0,-3.3134938367,5.6309288389,-0.7868767281\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-322.4166353\MP4/GTBas1=-322.5210979\CSD(T)/G3Bas1=-322.5338252\MP2/GTBas2=-322.4271759\MP4/GTBas2=-322.532186\MP2/GTBas3=-322.6118981\MP4/GTBas3=-322.7269283\HF/GTLargeXP=-321.5759722\MP2/GTLargeXP=-323.0740327\HF/GFHFB1=-321.600905\HF/GFHFB2=-321.6052365\G4=-323.2760411\FreqCoord=-5.6740284005,5.8411195468,-1.0073237575,-7.5721991708,4.131627165,-1.8453023056,-3.3514041794,4.9222134579,0.1424772395,-2.9365677829,2.3719937675,0.4464634246,-7.0193766491,1.6573260742,-1.4784014266,-4.8027329222,0.6574577343,-0.3759869765,-1.9637361865,6.302972643,0.7496710831,-4.5497404735,-1.3699042711,-0.1710851793,-1.2077149955,1.6835863043,1.302503785,-9.3056590335,4.808140793,-2.7030564738,-6.0020361217,8.4592276342,-1.2725536414,-6.2615958943,10.6409133794,-1.4869815164\PG=C01 [X(C7H4N1)]\NImag=0\\

³o-cyanophenyl cation

\1,3\C,0,-2.7679275795,2.8685033676,-0.3366486961\C,0,-3.9877217799,2.1239729746,-0.2468758638\C,0,-1.5650900384,2.1396088317,-0.5459521432\C,0,-1.6429621186,0.7708293803,-0.6492919523\C,0,-4.1083870865,0.7739160072,-0.3433644358\C,0,-2.9013941568,0.0813841873,-0.5501815391\C,0,-2.7824983813,4.2645473141,-0.2195965187\H,0,-0.6220624396,2.6690324406,-0.6191675108\H,0,-5.0582761657,0.2563970295,-0.2683154342\H,0,-2.9127303872,-1.0016422602,-0.6381813762\H,0,-0.7435950795,0.1861379867,-0.809065922\N,0,-2.789644788,5.4288127413,-0.1225986171\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-322.4173183\MP4/GTBas1=-322.5214769\CCSD(T)/G3Bas1=-322.5330577\MP2/GTBas2=-322.4277975\MP4/GTBas2=-322.5324998\MP2/GTBas3=-322.61243\MP4/GTBas3=-322.7271258\HF/GTLargeXP=-321.5750138\MP2/GTLargeXP=-323.0744901\HF/GFHFB1=-321.5999793\HF/GFHFB2=-321.6043099\G4=-323.2748763\FreqCoord=-5.2306250809,5.420685776,-0.6361738386,-7.5357020582,4.0137272355,-0.4665277708,-2.957591546,4.0432747235,-1.0317000323,-3.1047484508,1.456656424,-1.2269839702,-7.7637264415,1.4624893035,-0.6488647474,-5.4828403599,0.1537938256,-1.0396924323

, -5.2581599058, 8.0588265044, -0.4149772797, -1.1755276485, 5.0437403525, -1.1700570259, -9.5587566578, 0.484520167, -0.5070426878, -5.5042627307, -1.892829555, -1.2059880241, -1.4051910541, 0.3517498178, -1.528913016, -5.2716646574, 10.2589693078, -0.2316778106\PG=C01 [X(C7H4N1)]\NImag=0\

³p-cyanophenyl cation

\\1,3\C,0,-2.7557101386,2.9892263301,0.\C,0,-3.9727065697,2.220948626,0.\C,0,-1.5505746354,2.3289222573,0.\C,0,-1.6226007602,0.9294469372,0.\C,0,-3.9688335792,0.781740972,0.\C,0,-2.7653680937,0.1183977315,0.\C,0,-5.2004980576,2.8956802039,0.\H,0,-2.8136574177,4.0723853339,0.\H,0,-0.6019473866,2.8544311678,0.\H,0,-4.9142581433,0.2499855185,0.\H,0,-2.700430572,-0.9641162722,0.\N,0,-6.2251046462,3.4587511941,0.\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-322.4275431\MP4/GTBas1=-322.529721\CCSD(T)/G3Bas1=-322.5385597\MP2/GTBas2=-322.4381013\MP4/GTBas2=-322.5407484\MP2/GTBas3=-322.6224139\MP4/GTBas3=-322.7351303\HF/GTLargeXP=-321.5797707\MP2/GTLargeXP=-323.0847708\HF/GFHFB1=-321.6046925\HF/GFHFB2=-321.6090195\G4=-323.279859\FreqCoord=-5.2075374635,5.6488191131,0.,-7.507327423,4.1969846584,0.,-2.9301614095,4.4010252511,0.,-3.0662710598,1.7564001663,0.,-7.5000085317,1.4772763439,0.,-5.2257883536,0.2237392873,0.,-9.8275170835,5.4720425537,0.,-5.3170419512,7.6956929887,0.,-1.1375157071,5.3940931724,0.,-9.2866020371,0.4724041671,0.,-5.103074222,-1.8219157148,0.,-11.7637429298,6.5360925186,0.\PG=CS [SG(C7H4N1)]\NImag=0\

³m-bromophenyl cation

\\1,3\C,0,-2.9972875559,2.8409104042,-0.4049144741\C,0,-3.9855469507,1.9295589075,-0.8710978777\C,0,-1.7558859414,2.3882365122,0.1645259299\C,0,-1.4962362585,1.0398625063,0.2709505058\C,0,-3.6488744751,0.6262503405,-0.7286025391\C,0,-2.4609245313,0.1126331239,-0.1844939799\H,0,-1.0385577546,3.1261416345,0.5036777005\H,0,-2.2885685826,-0.9571024025,-0.1156158908\H,0,-0.563758859,0.6888396907,0.6985738311\H,0,-4.9190502834,2.2760554508,-1.2992415466\Br,0,-3.2925900977,4.6536238038,-0.5231288692\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-2802.2353181\MP4/GTBas1=-2802.3172443\CCSD(T)/G3Bas1=-2802.3217237\MP2/GTBas2=-2802.2445092\MP4/GTBas2=-2802.3268132\MP2/GTBas3=-2802.423674\MP4/GTBas3=-2802.5200418\HF/GTLargeXP=-2801.6495616\MP2/GTLargeXP=-2803.8851823\HF/GFHFB1=-2801.7319343\HF/GFHFB2=-2801.7354142\G4=-2804.1168265\FreqCoord=-5.6640526222,5.3685426321,-0.7651774633,-7.5315922265,3.6463378925,-1.6461364237,-3.3181435497,4.5131129485,0.3109089493,-2.8274767587,1.9650553527,0.5120222516,-6.8953734511,1.1834416342,-1.3768592587,-4.6504733978,0.2128457577,-0.3486430951,-1.9625897294,5.9075515417,0.9518129132,-4.3247678574,-1.8086614219,-0.2184823702,-1.0653498484,1.3017183649,1.3201132243,-9.2956578696,4.3011214652,-2.4552107035,-6.2220935526,8.7940745146,-0.988570295\PG=C01 [X(C6H4Br1)]\NImag=0\

³o-bromophenyl cation

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\HF/GFHFB1=-2801.7344435\HF/GFHFB2=-2801.7379229\G4=-2804.1160396\Freq
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,0.9733870857,-0.2772709683,-7.6792857222,1.0564545256,-0.2104274215,-
5.3762413321,-0.2918528989,-0.1447638257,-1.0535673088,4.5423398942,-0
.5764688459,-9.486565213,0.0965243674,-0.1098978622,-5.411533101,-2.33
81564051,0.0099781217,-1.2789525404,-0.1464119454,-0.2196498302,-5.194
1993466,8.4030290989,-0.8027725686\PG=C01 [X(C6H4Br1)]\NImag=0\\

³p-bromophenyl cation

\1,3\C,0,-2.8241397621,3.0317485539,-0.2334398731\C,0,-4.018212340
6,2.2643958641,-0.0618321107\C,0,-1.6764001918,2.3873513023,-0.6405116
858\C,0,-1.786168495,1.0108866699,-0.8535349177\C,0,-4.0687997176,0.85
48702725,-0.2958162126\C,0,-2.9212058502,0.2102129251,-0.7028963198\H,
0,-2.8399121236,4.0988363531,-0.0424427539\H,0,-0.7426429394,2.9191501
602,-0.7866680496\H,0,-5.0005552723,0.3199065184,-0.1507273578\H,0,-2.
9016818962,-0.8569516379,-0.8948683456\Br,0,-5.5492514816,3.1242330983
,0.4812273018\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTbas1=-2802.237
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2827,1.9102989575,-1.6129472392,-7.6889171559,1.6154706942,-0.55901162
75,-5.5202790347,0.397244858,-1.3282815442,-5.3666561551,7.7456781708,
-0.0802051813,-1.40339177,5.5163943435,-1.4865871711,-9.4496799769,0.6
045357079,-0.284833427,-5.4833841087,-1.6194039048,-1.6910560981,-10.4
865655427,5.9039449311,0.9093878081\PG=C01 [X(C6H4Br1)]\NImag=0\\

³m-chlorophenyl cation

\1,3\C,0,-3.0003081355,2.855712621,-0.4061591303\C,0,-3.9897122879
,1.943222469,-0.8728829499\C,0,-1.7548545492,2.398680361,0.1651106301\
C,0,-1.4962098157,1.0521811239,0.2710894619\C,0,-3.6546537644,0.641010
3502,-0.7311227903\C,0,-2.4634031124,0.1260851778,-0.1855014905\H,0,-1
.0415498064,3.1418360525,0.5024548527\H,0,-2.2931286216,-0.9442963239,
-0.1175924998\H,0,-0.5644643513,0.6990217321,0.6983523851\H,0,-4.92107
971,2.2972975204,-1.2999620924\Cl,0,-3.2679562997,4.5142589059,-0.5131
453943\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTbas1=-689.4792239\MP4
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-3.3161945011,4.5328489627,0.3120138727,-2.8274267891,1.9883341663,0.5
122848405,-6.9062947253,1.2113340103,-1.3816218432,-4.6551572374,0.238
2664555,-0.3505470144,-1.9682438878,5.9372096937,0.9495020658,-4.33338
50824,-1.7844614405,-0.2222176198,-1.0666830358,1.3209596346,1.3196947
52,-9.2994929301,4.3412631593,-2.4565723377,-6.1755424206,8.5307130251
, -0.9697042616\PG=C01 [X(C6H4Cl1)]\NImag=0\\

³o-chlorophenyl cation

\1,3\C,0,-2.7248844069,2.633587877,-0.2885599595\C,0,-3.9475684052
,1.9189419228,-0.2156327696\C,0,-1.5060734665,1.8962411273,-0.25201654
67\C,0,-1.5832907528,0.5307884428,-0.1479252504\C,0,-4.0665922866,0.57
14495427,-0.11224211\C,0,-2.8467509761,-0.1416677625,-0.0775423519\H,0
, -0.5599500553,2.4226661988,-0.3064441157\H,0,-5.0224799634,0.06226040

81,-0.0589599708\H,0,-2.8636798054,-1.2246357683,0.0043234225\H,0,-0.6
76196081,-0.0625025306,-0.1173739934\C1,0,-2.7351237945,4.3064305724,-
0.4144459478\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-689.47673
94\MP4/GTBas1=-689.5706708\CCSD(T)/G3Bas1=-689.5775003\MP2/GTBas2=-689
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FB1=-688.7934724\HF/GFHFB2=-688.7980149\G4=-690.5645713\FreqCoord=-5.1
492852728,4.9767598345,-0.5452992964,-7.4598231766,3.6262746991,-0.407
4868798,-2.8460663877,3.5833764126,-0.4762422542,-2.9919859116,1.00304
47914,-0.2795382113,-7.6847457157,1.0798831344,-0.2121068485,-5.379579
7134,-0.2677132729,-0.1465338088,-1.0581522526,4.5781756271,-0.5790954
536,-9.4911116387,0.1176551202,-0.1114181976,-5.4115705645,-2.31422621
46,0.0081700844,-1.2778254053,-0.1181126654,-0.2218047027,-5.168634911
1,8.1379743921,-0.7831893383\PG=C01 [X(C6H4C11)]\NImag=0\\

³p-chlorophenyl cation

\\1,3\C,0,-2.8326978265,3.0402371075,-0.2297596631\C,0,-4.029004768
9,2.2704575968,-0.0580027878\C,0,-1.6869721917,2.3968236771,-0.6361443
176\C,0,-1.7983510726,1.0177295877,-0.8492151936\C,0,-4.0805426255,0.8
5778113,-0.2922950674\C,0,-2.9348361002,0.214332782,-0.6986814546\H,0,
-2.8562744205,4.1069835907,-0.036821879\H,0,-0.751929565,2.9260364637,
-0.7830842161\H,0,-5.0160145756,0.3296311071,-0.1450583426\H,0,-2.9124
077881,-0.8525953781,-0.8913559809\C1,0,-5.429939095,3.0572217973,0.43
89096716\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-689.4817277\M
P4/GTBas1=-689.5754852\CCSD(T)/G3Bas1=-689.5823807\MP2/GTBas2=-689.490
7106\MP4/GTBas2=-689.5848914\MP2/GTBas3=-689.6801788\MP4/GTBas3=-689.7
898333\HF/GTLargeXP=-688.7707645\MP2/GTLargeXP=-690.3764995\HF/GFHFB1=
-688.7983425\HF/GFHFB2=-688.8028781\G4=-690.569447\FreqCoord=-5.353023
1093,5.7452155123,-0.4341828396,-7.6137156013,4.2905430543,-0.10960938
4,-3.1879154361,4.5293403385,-1.2021385413,-3.3983910181,1.9232301982,
-1.6047841438,-7.7111080357,1.6209714176,-0.5523576273,-5.5460364743,0
.4050302594,-1.3203166033,-5.397576415,7.7610742186,-0.0695832669,-1.4
20940949,5.5294075712,-1.4798147075,-9.4788938264,0.6229125173,-0.2741
205408,-5.5036531069,-1.6111717668,-1.6844186908,-10.2610978078,5.7773
119244,0.8294190764\PG=C01 [X(C6H4C11)]\NImag=0\\

³m-ethynylphenyl cation

\\1,3\C,0,-2.9970339803,2.9141113105,-0.4037018608\C,0,-3.9870064951,1
.9799056066,-0.8720683059\C,0,-1.7604185492,2.4324056638,0.1640507876\
C,0,-1.5125569692,1.084089904,0.2647161659\C,0,-3.6660490042,0.6740435
341,-0.7370990354\C,0,-2.4840944191,0.1625639739,-0.1949753928\H,0,-1.
0357826836,3.1613053814,0.5073548231\H,0,-2.3107184943,-0.907326538,-0
.1258907057\H,0,-0.5842451151,0.7214309253,0.6909132054\H,0,-4.9171771
631,2.3364820692,-1.2991894031\C,0,-3.2237669559,4.2770975493,-0.49443
16021\C,0,-3.4273794131,5.4783510116,-0.5761440963\H,0,-3.6053207578,6
.5300296084,-0.64756458\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1
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TBas2=-306.380869\MP4/GTBas2=-306.4849149\MP2/GTBas3=-306.5683147\MP4/
GTBas3=-306.6821104\HF/GTLargeXP=-305.5441312\MP2/GTLargeXP=-307.02102
82\HF/GFHFB1=-305.5681542\HF/GFHFB2=-305.5723233\G4=-307.2067264\FreqC
oord=-5.6635734338,5.5068722975,-0.7628859562,-7.5343503658,3.74147936
54,-1.6479702673,-3.3267089372,4.5965805486,0.3100110604,-2.8583184322
,2.0486330221,0.5002410565,-6.9278286076,1.273757681,-1.3929153096,-4.
6942581402,0.3072013897,-0.368450095,-1.9573456052,5.9740013933,0.9587
616679,-4.3666251244,-1.7145986699,-0.2378989565,-1.104063262,1.363306
8726,1.3056367399,-9.2921181852,4.4153112252,-2.4551121666,-6.09203666
29,8.0825430119,-0.9343403193,-6.4768084443,10.3525830717,-1.088754555

1,-6.8130688534,12.3399675996,-1.2237197096\PG=C01 [X(C8H5)]\NImag=0\\

³o-ethynylphenyl cation

\\1,3\C,0,-2.7054447853,2.7289280084,-0.2589200825\C,0,-3.9289286347,2.0070671557,-0.1971395713\C,0,-1.49470799,1.9546226694,-0.2368485245\C,0,-1.5788339154,0.5884290547,-0.1591204012\C,0,-4.0537144156,0.6581588872,-0.1196558519\C,0,-2.841298598,-0.0661868758,-0.1004764417\H,0,-0.5419976347,2.4694356034,-0.2822456275\H,0,-5.0123198027,0.153805794,-0.0746921654\H,0,-2.8726207803,-1.150229879,-0.0394066111\H,0,-0.6762305376,-0.0113972758,-0.1414355191\C,0,-2.6911573949,4.109901941,-0.3361848394\C,0,-2.676086387,5.3287221069,-0.4044243136\H,0,-2.6662791239,6.39610281,-0.464110051\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-306.3644076\MP4/GTBas1=-306.4700208\CCSD(T)/G3Bas1=-306.4842825\MP2/GTBas2=-306.3755684\MP4/GTBas2=-306.4813515\MP2/GTBas3=-306.5609666\MP4/GTBas3=-306.677126\HF/GTLargeXP=-305.5496794\MP2/GTLargeXP=-307.014065\HF/GFHFB1=-305.5737478\HF/GFHFB2=-305.5779243\G4=-307.2058993\FreqCoord=-5.1125497119,5.1569265723,-0.4892880461,-7.4245991152,3.7928072545,-0.3725397997,-2.8245887497,3.6937015382,-0.4475788464,-2.9835637094,1.111969762,-0.3006939804,-7.6604100663,1.2437400487,-0.2261167902,-5.369276212,-0.1250750689,-0.1898729577,-1.0242270942,4.6665569932,-0.5333669381,-9.4719117176,0.2906508283,-0.1411477368,-5.4284665584,-2.1736194612,-0.0744677027,-1.2778905188,-0.0215377298,-0.2672743965,-5.0855504569,7.7665891016,-0.6352972765,-5.0570703793,10.0698254203,-0.7642511941,-5.0385373379,12.0868826286,-0.8770408918\PG=C01 [X(C8H5)]\NImag=0\\

³p-ethynylphenyl cation

\\1,3\C,0,-2.9446984141,3.0784583139,-0.211275812\C,0,-4.1497903145,2.3085204707,-0.0534138118\C,0,-1.7804927329,2.447474277,-0.5874365683\C,0,-1.8708808438,1.0708633047,-0.7901490079\C,0,-4.1573060577,0.8881856738,-0.2827002478\C,0,-2.9941929887,0.2552246922,-0.6589259115\H,0,-2.9768129233,4.1469799552,-0.0298940044\H,0,-0.8500100775,2.9884028476,-0.7180336965\H,0,-5.0842091926,0.3404980026,-0.1540240428\H,0,-2.9543996187,-0.8126523804,-0.8419879692\C,0,-5.3207690833,2.9444862846,0.3251619835\C,0,-6.3526339226,3.5049915044,0.6587406574\H,0,-7.2561838304,3.9955270536,0.9514184312\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-306.3703293\MP4/GTBas1=-306.4752615\CCSD(T)/G3Bas1=-306.48892\MP2/GTBas2=-306.3814728\MP4/GTBas2=-306.4865398\MP2/GTBas3=-306.5671409\MP4/GTBas3=-306.6825312\HF/GTLargeXP=-305.5542138\MP2/GTLargeXP=-307.0203779\HF/GFHFB1=-305.5782541\HF/GFHFB2=-305.5824273\G4=-307.2106024\FreqCoord=-5.5646735465,5.8174431248,-0.3992534231,-7.8419672033,4.3624714618,-0.1009374761,-3.3646436467,4.6250561008,-1.1100942345,-3.535452422,2.0236383717,-1.4931652291,-7.8561698995,1.6784276787,-0.534226046,-5.6582047376,0.4823047707,-1.2451895145,-5.6253611739,7.8366563939,-0.0564914813,-1.6062862567,5.6472629567,-1.3568870405,-9.6077629762,0.6434479736,-0.2910632588,-5.5830061665,-1.5356904403,-1.5911266691,-10.0547963839,5.56427268,0.6144670977,-12.0047383362,6.6234740414,1.2448394351,-13.7122002094,7.5504518878,1.7979202728\PG=C01 [X(C8H5)]\NImag=0\\

³m-(dimethylamino)phenyl cation

\\1,3\C,0,-2.8818900279,2.6365199841,-0.4811291899\C,0,-3.9154196561,1.677506334,-0.7662706988\C,0,-1.6567606372,2.167366454,0.0987478769\C,0,-1.4657056107,0.8315980666,0.3782654589\C,0,-3.6475300731,0.3883727061,-0.4506984857\C,0,-2.4828823386,-0.1093472698,0.1118739795\H,0,-0.8510887545,2.8619051034,0.290978321\H,0,-2.3505187532,-1.1612281299,0.3397254507\H,0,-0.5255275205,0.5003898035,0.8051010268\N,0,-3.059378

7871,3.9490882506,-0.7605791801\C,0,-2.1244436197,4.9878523101,-0.3135
575492\C,0,-4.2095854622,4.4299348631,-1.5336241739\H,0,-1.6830858723,
4.7288428621,0.6467427163\H,0,-2.6773307123,5.9213500425,-0.2046052602
\H,0,-1.3358581414,5.1327039657,-1.0610697756\H,0,-5.0693847327,4.5887
495072,-0.8723713172\H,0,-4.4722548714,3.7214677476,-2.3177759559\H,0,
-3.9421239508,5.3809063367,-1.9940162594\H,0,-4.8697604784,1.975651062
1,-1.180166984\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-364.012
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FHFb1=-363.05509\HF/GFHFb2=-363.0604736\G4=-365.0144713\FreqCoord=-5.4
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0417645,-3.130823872,4.0957290277,0.1866064435,-2.7697821957,1.5714925
986,0.7148181228,-6.8928328996,0.7339180521,-0.8516967065,-4.691967640
2,-0.2066363933,0.2114111826,-1.6083246607,5.4082168637,0.5498693372,-
4.4418367137,-2.1944031432,0.6419880622,-0.993103089,0.9455996883,1.52
142045,-5.7813880444,7.4626952682,-1.4372863528,-4.014616626,9.4256748
575,-0.5925378949,-7.9549636566,8.3713636778,-2.8981296795,-3.18057135
67,8.9362179349,1.2221666122,-5.0594218134,11.1897299173,-0.386647907,
-2.5244060396,9.6994048164,-2.0051312837,-9.5797488071,8.6714798611,-1
.6485428757,-8.4513369034,7.0325548554,-4.379961794,-7.4495346488,10.1
684393231,-3.7681446348,-9.2025136369,3.7334394415,-2.2301923908\PG=C0
1 [X(C8H10N1)]\NImag=0\\

³o-(dimethylamino)phenyl cation

\\1,3\C,0,-2.8436053931,2.6618553733,-0.4812453253\C,0,-3.833152054
6,1.6871069003,-0.739032293\C,0,-1.6398226991,2.1803541473,0.134411282
1\C,0,-1.5180291438,0.8433985821,0.4301133166\C,0,-3.7486798466,0.3604
508649,-0.4615658383\C,0,-2.5517138053,-0.0751723897,0.1427871729\H,0,
-0.8335760133,2.8654091677,0.3641909211\H,0,-4.5495664158,-0.334932063
4,-0.6870906802\H,0,-2.4260951889,-1.1244394001,0.3880128643\H,0,-0.60
7535125,0.4835770797,0.894972408\N,0,-3.036029551,3.9555218252,-0.8001
335753\C,0,-2.0175460871,4.9764562333,-0.5379276017\C,0,-4.2752458183,
4.4141345314,-1.4272310798\H,0,-1.8049160611,5.0334176875,0.5332615118
\H,0,-2.3948617725,5.9392629579,-0.8776119158\H,0,-1.0971880752,4.7417
122553,-1.0799159055\H,0,-4.9541740517,3.5752364521,-1.5736306021\H,0,
-4.0388901458,4.875068781,-2.3915906331\H,0,-4.7445727518,5.1658110143
, -0.7845640267\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-364.013
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FHFb1=-363.0767232\HF/GFHFb2=-363.082117\G4=-365.0204662\FreqCoord=-5.
3736354229,5.0301776609,-0.9094218675,-7.2436076088,3.1881699985,-1.39
65686372,-3.0988158079,4.120272211,0.2540005124,-2.8686593436,1.593792
3411,0.8127963745,-7.0839782699,0.681153419,-0.8722330267,-4.822040261
5,-0.1420552293,0.269828652,-1.5752303761,5.4148385856,0.6882211009,-8
.5974345493,-0.632929873,-1.298413214,-4.5846554794,-2.1248825192,0.73
32380496,-1.1480750023,0.9138282447,1.6912527476,-5.7372643827,7.47485
29623,-1.512033327,-3.812609565,9.4041393932,-1.0165358464,-8.07904374
74,8.3415053781,-2.6970758692,-3.4107970482,9.5117809418,1.0077182145,
-4.5256328762,11.2235804217,-1.6584461718,-2.0733849784,8.9605375635,-
2.040745308,-9.3620321723,6.7562177548,-2.9737308723,-7.6323962564,9.2
12544875,-4.5194513186,-8.9659431185,9.7619680712,-1.4826111442\PG=C01
[X(C8H10N1)]\NImag=0\\

³p-(dimethylamino)phenyl cation

\\1,3\C,0,-2.8494507091,2.9962350692,-0.1146935006\C,0,-4.076937252

7,2.2562810798,-0.0458632757\C,0,-1.6645173323,2.352031974,-0.40809327
14\C,0,-1.7326570704,0.9865462053,-0.6394614961\C,0,-4.060822657,0.842
7834068,-0.2921961415\C,0,-2.876437428,0.2037081783,-0.5987320543\H,0,
-2.837261887,4.0561075065,0.1009686787\H,0,-0.7279249254,2.8967383603,
-0.4440230328\H,0,-4.9813108422,0.2748792522,-0.2780199268\H,0,-2.8543
684185,-0.8602542006,-0.8053863506\N,0,-5.238336782,2.8852067411,0.248
4109117\C,0,-5.3502186963,4.3476730629,0.2962163748\C,0,-6.4759247455,
2.1532093742,0.542008306\H,0,-7.0130440236,1.9281197512,-0.3865352246\
H,0,-7.1078670061,2.7851910948,1.1660764406\H,0,-6.2638355525,1.231359
0799,1.080772785\H,0,-4.7140958649,4.8111627677,-0.4558071587\H,0,-5.0
803731715,4.716515323,1.2924724691\H,0,-6.3862356352,4.6188359734,0.09
28054671\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-364.0094572\M
P4/GTBas1=-364.1391176\CCSD(T)/G3Bas1=-364.1608323\MP2/GTBas2=-364.023
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240717\HF/GTLargeXP=-363.0433013\MP2/GTLargeXP=-364.809745\HF/GFHFB1=-
363.0717802\HF/GFHFB2=-363.0771675\G4=-365.0165908\FreqCoord=-5.384681
4693,5.6620637105,-0.2167393054,-7.7042948685,4.2637533197,-0.08666903
07,-3.1454819015,4.4446962866,-0.7711845197,-3.2742473452,1.8643021455
, -1.2084071001,-7.6738426959,1.5926298281,-0.5521706845,-5.4356789772,
0.384952668,-1.1314396097,-5.3616479337,7.6649323528,0.1908031508,-1.3
755787543,5.4740421795,-0.8390819286,-9.4133132744,0.5194465062,-0.525
3815212,-5.3939745933,-1.6256448438,-1.5219596338,-9.8990219098,5.4522
505775,0.4694285916,-10.110448087,8.2159114042,0.5597678245,-12.237724
2261,4.0689760241,1.02424726,-13.2527325625,3.6436182811,-0.7304457151
, -13.4319220306,5.263248397,2.2035651228,-11.8369337356,2.3269314323,2
.0423645756,-8.9083501488,9.0917800118,-0.8613506994,-9.600513947,8.91
29222619,2.4424190009,-12.0682363705,8.7283350424,0.1753769165\PG=C01
[X(C8H10N1)]\NImag=0\\

³syn-m-thiomethoxyphenyl cation

\\1,3\C,0,0.3075302504,1.2114394396,0.0000221904\C,0,1.6467976482,1.4
270000391,0.0001038764\C,0,2.6510366872,0.4644922094,0.0001139566\C,0,
2.2477750728,-0.8846594831,0.0000048338\C,0,0.9020671516,-1.194450014,
-0.0000864373\C,0,-0.087046425,-0.1581285315,-0.0000762197\H,0,-0.4138
930038,2.0184436445,-0.000016554\H,0,3.7017488917,0.7354250415,0.00019
30725\H,0,2.9904122817,-1.6744383463,-0.0000037942\H,0,0.5793404108,-2
.2302336047,-0.0001746545\S,0,-1.7049756354,-0.7206126683,-0.000229934
9\C,0,-2.7661826184,0.7461483559,0.000108013\H,0,-2.5931697238,1.33709
44828,-0.901645403\H,0,-3.7862647723,0.3586019594,-0.0008349811\H,0,-2
.5943882159,1.3358674757,0.9028910207\\Version=EM64L-G09RevB.01\State=
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.5261463\MP4/GTBas3=-667.6543784\HF/GTLargeXP=-666.4557515\MP2/GTLarge
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696783\FreqCoord=0.5811479509,2.2892887674,0.0000419337,3.1119965514,2
.6966392655,0.0001962979,5.009733307,0.8777630665,0.0002153468,4.24767
92959,-1.6717641439,0.0000091346,1.7046598701,-2.257183406,-0.00016334
29,-0.1644939041,-0.2988196183,-0.0001440344,-0.7821444255,3.814305702
8,-0.0000312825,6.995291618,1.3897519197,0.0003648542,5.6510602369,-3.
1642299009,-0.00000717,1.094794714,-4.2145307253,-0.0003300493,-3.2219
370141,-1.361760591,-0.0004345139,-5.2273275823,1.4100160472,0.0002041
15,-4.900380594,2.5267423863,-1.7038628806,-7.1550034862,0.677659494,-
0.0015778857,-4.9026832104,2.524423679,1.706216757\PG=C01 [X(C7H7S1)]\
NImag=0\\

³syn-o-thiomethoxyphenyl cation

\\1,3\C,0,0.8345047317,-1.2864220919,0.0000123339\C,0,-0.144356751,-0

.238942352,0.0000671438\C,0,0.3301072595,1.0785482291,0.0001348146\C,0
,1.6372819608,1.4508807519,0.0001502544\C,0,2.5802651046,0.397883163,0
.0000992712\C,0,2.1690533194,-0.9524126298,0.0000285945\H,0,0.51113260
7,-2.3223986486,-0.0000437328\H,0,1.9551470203,2.4874514809,0.00019737
4\H,0,3.6391504199,0.6364869313,0.0001089865\H,0,2.9185065331,-1.73511
45894,-0.0000141067\S,0,-1.7944293416,-0.673330563,0.0000295561\C,0,-2
.6918101192,0.9025379238,0.0001495506\H,0,-2.440833381,1.4670880997,-0
.8995160431\H,0,-3.7495033318,0.6355699826,-0.0000829776\H,0,-2.441161
0317,1.4667143127,0.9001469807\\Version=EM64L-G09RevB.01\State=3-A\MP2
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\MP2/GTBas2=-667.2879257\MP4/GTBas2=-667.4045132\MP2/GTBas3=-667.51413
88\MP4/GTBas3=-667.6465286\HF/GTLargeXP=-666.4718762\MP2/GTLargeXP=-66
8.2587951\HF/GFHFB1=-666.4998751\HF/GFHFB2=-666.5057704\G4=-668.472425
1\FreqCoord=1.5769853995,-2.430985445,0.0000233077,-0.2727947249,-0.45
15356069,0.0001268835,0.6238123149,2.0381607741,0.0002547626,3.0940145
082,2.7417672725,0.0002839396,4.875994398,0.7518902109,0.0001875953,4.
0989167413,-1.7997990359,0.0000540358,0.9659006449,-4.3886974173,-0.00
0082643,3.6946924179,4.7006020678,0.0003729828,6.87699765,1.2027859873
,0.0002059547,5.5151780646,-3.278891383,-0.0000266579,-3.3909800204,-1
.272410361,0.0000558529,-5.086783927,1.7055495004,0.0002826096,-4.6125
066262,2.7723947212,-1.6998389737,-7.0855344314,1.2010532054,-0.000156
805,-4.6131257962,2.7716883661,1.7010312729\PG=C01 [X(C7H7S1)]\NImag=0
\\

³p-thiomethoxyphenyl cation

\\1,3\C,0,0.3633432208,1.1638364492,0.0000018944\C,0,1.713602606,1.45
92189447,0.0000022231\C,0,2.5896614445,0.3797593135,0.0000010999\C,0,2
.259523274,-0.9661698808,-0.0000003076\C,0,0.9092258847,-1.2609194506,
-0.0000006257\C,0,-0.0503564944,-0.1979638336,0.0000004001\H,0,-0.3664
737745,1.9634020684,0.0000029534\H,0,2.0658119597,2.4847451511,0.00000
33758\H,0,3.0093491247,-1.7490179998,-0.0000010813\H,0,0.5668559045,-2
.2912092425,-0.0000016646\S,0,-1.6788584794,-0.7214129372,-0.000000141
8\C,0,-2.7178343672,0.7626800438,-0.000001911\H,0,-2.5398564287,1.3503
098464,-0.9026205665\H,0,-3.7423729911,0.386806099,0.0000024353\H,0,-2
.5398508838,1.3503154284,0.9026119168\\Version=EM64L-G09RevB.01\State=
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7.5158629\MP4/GTBas3=-667.6473103\HF/GTLargeXP=-666.4705029\MP2/GTLarg
eXP=-668.2605845\HF/GFHFB1=-666.4985191\HF/GFHFB2=-666.5044198\G4=-668
.4716747\FreqCoord=0.6866191795,2.1993321524,0.0000035798,3.238239626,
2.7575241734,0.0000042011,4.8937509071,0.7176410989,0.0000020785,4.269
8801788,-1.8257964726,-0.0000005813,1.718187915,-2.3827924372,-0.00000
11825,-0.0951599835,-0.3740974297,0.000000756,-0.6925350687,3.71029219
8,0.00000055811,3.9038188459,4.6954878456,0.0000063793,5.686845684,-3.3
05165021,-0.0000020433,1.0712024163,-4.3297579815,-0.0000031457,-3.172
582742,-1.36327288,-0.0000002681,-5.1359626286,1.4412564098,-0.00000036
113,-4.799633067,2.5517158042,-1.7057056726,-7.0720600402,0.7309575936
,0.000004602,-4.7996225887,2.5517263528,1.705689327\PG=C01 [X(C7H7S1)]
\NImag=0\\

³syn-m-methoxyphenyl cation

\\1,3\C,0,-1.2704218276,1.4026830375,0.0000255209\C,0,0.0599309301,1.
1720673711,0.0000249552\C,0,0.4238038553,-0.2128437795,-0.0000027432\C
,0,-0.5929251056,-1.2414738177,-0.0000208332\C,0,-1.9268748398,-0.9103
458421,-0.0000218542\C,0,-2.3027417038,0.4508867037,0.0000070044\H,0,0
.8010368747,1.9615609077,0.0000520437\H,0,-0.2529041908,-2.2705527983,
-0.0000400679\H,0,-2.6871476092,-1.6830024939,-0.0000427722\H,0,-3.346

4724642,0.7476504653,-0.0000000214\O,0,1.6445206657,-0.6642497762,-0.000099716\C,0,2.797942928,0.2203226727,-0.0000414702\H,0,2.784235361,0.8354678446,0.9022524242\H,0,3.6588918218,-0.4438924346,-0.0002059901\H,0,2.7840503043,0.8356799398,-0.9021862244\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-344.6686239\MP4/GTBas1=-344.7732942\CCSD(T)/G3Bas1=-344.778605\MP2/GTBas2=-344.6814173\MP4/GTBas2=-344.7870675\MP2/GTBas3=-344.909892\MP4/GTBas3=-345.0283887\HF/GTLargeXP=-343.7899929\MP2/GTLargeXP=-345.3943668\HF/GFHFB1=-343.8174548\HF/GFHFB2=-343.8226882\G4=-345.5759532\FreqCoord=-2.4007493274,2.650686792,0.0000482275,0.1132530448,2.2148863407,0.0000471585,0.8008732206,-0.4022164523,-0.000005184,-1.120466067,-2.3460455167,-0.000039369,-3.6412657395,-1.7203043277,-0.0000412985,-4.3515511749,0.8520523869,0.0000132365,1.5137403156,3.7068129085,0.0000983483,-0.4779196584,-4.290722959,-0.0000757174,-5.0779730601,-3.1804137944,-0.0000808278,-6.3239164685,1.4128546225,-0.000000404,3.1076936781,-1.2552501609,-0.0000188436,5.2873458693,0.4163495122,-0.0000783673,5.2614423219,1.5788054191,1.7050099845,6.914303493,-0.8388351339,-0.0003892649,5.2610926152,1.5792062209,-1.704884885\PG=C01 [X(C7H7O1)]\NImag=0\\

³syn-o-methoxyphenyl cation

\\1,3\C,0,-1.2888139833,1.4275274467,-0.0006786727\C,0,0.0148128486,1.0672088517,-0.0012472669\C,0,0.4883194497,-0.27119726,-0.0008103408\C,0,-0.4941928464,-1.3242836077,0.0003625948\C,0,-1.8215014662,-0.9919420537,0.000964146\C,0,-2.2359320288,0.367626256,0.0005215453\H,0,-1.6139010831,2.4624731529,-0.0004620114\H,0,-0.140613594,-2.3494965387,0.004437735\H,0,-2.5748882408,-1.7710246897,0.00169012\H,0,-3.2950026002,0.6056262458,0.0014821169\O,0,1.73601705,-0.6150007574,-0.0018342466\C,0,2.7846205378,0.3997366476,0.0020718807\H,0,2.7326534484,0.9560794419,0.9401392763\H,0,3.7148625762,-0.1581821155,-0.0717709384\H,0,2.6489839322,1.0601719799,-0.8564139768\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-344.6602029\MP4/GTBas1=-344.76772\CCSD(T)/G3Bas1=-344.7804869\MP2/GTBas2=-344.6728815\MP4/GTBas2=-344.7814847\MP2/GTBas3=-344.9004036\MP4/GTBas3=-345.0222572\HF/GTLargeXP=-343.7996181\MP2/GTLargeXP=-345.3842901\HF/GFHFB1=-343.8271326\HF/GFHFB2=-343.8323704\G4=-345.5770882\FreqCoord=-2.4355054647,2.6976359215,-0.0012825055,0.0279922271,2.0167324564,-0.0023569928,0.9227900254,-0.5124885493,-0.0015313221,-0.9338891366,-2.5025333408,0.0006852048,-3.4421389218,-1.8744988212,0.0018219719,-4.2252991862,0.6947129431,0.0009855778,-3.0498310527,4.6533998687,-0.0008730751,-0.2657211833,-4.4399050083,0.0008386104,-4.8658335979,-3.3467516381,0.0031938639,-6.2266525216,1.1444677435,0.0028007951,3.2805967865,-1.1621830029,-0.0034662237,5.2621702004,0.7553927892,0.003915287,5.1639666336,1.8067283065,1.776605759,7.0200728903,-0.2989208775,-0.1356274178,5.0058541622,2.0034346958,-1.6183878726\PG=C01 [X(C7H7O1)]\NImag=1\\

³p-methoxyphenyl cation

\\1,3\C,0,-1.3438663267,1.4404249642,0.0000961923\C,0,-0.0043188821,1.1297155964,0.0000789405\C,0,0.3790529627,-0.2518522057,0.0000141976\C,0,-0.6027572824,-1.307339517,-0.0000240038\C,0,-1.9399196721,-0.990770196,-0.0000108441\C,0,-2.2449752406,0.368911185,0.0000442487\H,0,-1.6872225868,2.4690555238,0.0001544433\H,0,0.7468549147,1.9091076751,0.0001392183\H,0,-0.242745317,-2.3302306027,-0.0000677747\H,0,-2.7089422148,-1.7547645923,-0.0000416415\O,0,1.6122295453,-0.6692583765,-0.0000110906\C,0,2.7498063153,0.2362167274,-0.0000813619\H,0,2.7277940008,0.8503883631,0.902477003\H,0,3.6212327219,-0.4142504695,-0.000351668\H,0,2.7274730617,0.8507149246,-0.9024048591\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-344.6639848\MP4/GTBas1=-344.7706359\CCSD(T)/G3Bas1=-3

44.7821295\MP2/GTbas2=-344.6766859\MP4/GTbas2=-344.7843587\MP2/GTbas3=-344.9040881\MP4/GTbas3=-345.025\HF/GTLargeXP=-343.8008883\MP2/GTLargeXP=-345.3884148\HF/GFHFB1=-343.8283739\HF/GFHFB2=-343.833614\G4=-345.5782287\FreqCoord=-2.5395393166,2.7220086973,0.0001817771,-0.0081615044,2.1348530853,0.0001491759,0.7163062894,-0.4759316947,0.0000268296,-1.1390461884,-2.4705136498,-0.0000453606,-3.6659169001,-1.8722843311,-0.0000204925,-4.2423883798,0.6971411071,0.000083618,-3.1883886143,4.6658387468,0.0002918556,1.4113512499,3.6076906641,0.0002630845,-0.4587221692,-4.4034976656,-0.0001280757,-5.1191588958,-3.3160245071,-0.000078691,3.0466723041,-1.2647150438,-0.0000209582,5.1963808545,0.4463849228,-0.0001537517,5.1547836085,1.6070011128,1.7054343769,6.8431381078,-0.7828199378,-0.0006645563,5.1541771215,1.6076182247,-1.7052980446\PG=C01 [X(C7H7O1)]\NImag=0\

³anti-o-thiomethoxyphenyl cation

\1,3\C,0,-3.5477748017,3.67499296,-0.0031344862\C,0,-4.7187823172,2.9520133171,-0.0026070616\C,0,-2.3066696198,2.9712064846,-0.0008367655\C,0,-4.7139312344,1.5358003231,0.0001604167\C,0,-3.506428744,0.8129580573,0.0024863056\C,0,-2.3720372915,1.5651610607,0.0018646686\H,0,-5.6571588979,0.9987210573,0.0005077697\S,0,-0.7375510484,3.6455581069,-0.000963906\H,0,-3.5677352821,4.7577376173,-0.0052729305\H,0,-5.668736346,3.4740986844,-0.0043420144\C,0,-0.9611950066,5.4431196581,-0.0044933219\H,0,0.0495844995,5.8543995328,-0.0050898512\H,0,-1.4898199453,5.7595551846,0.8968894137\H,0,-1.4894528106,5.7560292392,-0.9073264606\H,0,-3.4940311541,-0.2709912833,0.0046182236\Version=EM64L-G09RevB.01\State=3-A\MP2/GTbas1=-667.2746303\MP4/GTbas1=-667.3903399\CCSD(T)/G3bas1=-667.4086795\MP2/GTbas2=-667.2861416\MP4/GTbas2=-667.4025701\MP2/GTbas3=-667.5125238\MP4/GTbas3=-667.6447394\HF/GTLargeXP=-666.4694001\MP2/GTLargeXP=-668.257285\HF/GFHFB1=-666.4973883\HF/GFHFB2=-666.5033019\G4=-668.4701603\FreqCoord=-6.7043227564,6.9447302347,-0.0059233205,-8.9172062603,5.5784967099,-0.0049266324,-4.3589738604,5.6147665401,-0.0015812576,-8.9080390422,2.9022420054,0.0003031436,-6.6261900307,1.5362680857,0.0046984367,-4.4825008579,2.9577257586,0.003523713,-10.6904810072,1.8873092814,0.0009595457,-1.3937694906,6.8891064236,-0.0018215183,-6.7420425979,8.9908211087,-0.0099643946,-10.7123592135,6.5650950721,-0.0082052181,-1.8163953228,10.2860054624,-0.0084911478,0.0937011245,11.0632117896,-0.0096184248,-2.815351684,10.8839819461,1.6948753634,-2.8146578999,10.8773188749,-1.7145985237,-6.602761981,-0.5120993098,0.0087271779\PG=C01 [X(C7H7S1)]\NImag=0\

³anti-o-methoxyphenyl cation

\1,3\C,0,-1.2500679472,1.4308532971,0.0035302566\C,0,0.0340144859,0.9940708909,0.0004857897\C,0,0.4489433614,-0.370690994,-0.0003813411\C,0,-0.580194037,-1.3676197916,0.0023885172\C,0,-1.8873749001,-0.9567903882,0.0055522247\C,0,-2.2408984567,0.4265390673,0.0061184449\H,0,-1.5126478034,2.4830026961,0.0039821685\H,0,-0.3245588785,-2.4198464949,0.0021504107\H,0,-2.6813144177,-1.6951044541,0.007743915\H,0,-3.2896787831,0.7061993473,0.0086102208\O,0,1.7273883014,-0.5931516034,-0.0034776393\C,0,2.2770699083,-1.9393014738,-0.0053013063\H,0,1.959604734,-2.4630050452,0.8989295104\H,0,3.3551101677,-1.7976300354,-0.0106095447\H,0,1.950874265,-2.4645050181,-0.9055116272\Version=EM64L-G09RevB.01\State=3-A\MP2/GTbas1=-344.658335\MP4/GTbas1=-344.7652442\CCSD(T)/G3bas1=-344.7768677\MP2/GTbas2=-344.6711463\MP4/GTbas2=-344.7790765\MP2/GTbas3=-344.8985617\MP4/GTbas3=-345.0197891\HF/GTLargeXP=-343.7963651\MP2/GTLargeXP=-345.382908\HF/GFHFB1=-343.823879\HF/GFHFB2=-343.829123\G4=-345.5734214\FreqCoord=-2.3622860678,2.7039208678,0.0066712182,0.0642780628,1.8785217405,0.0009180094,0.8483800022,-0.7005044586,-0.0007206302,-

1.0964078338,-2.58442686,0.0045136434,-3.5666216713,-1.8080718002,0.01
0492184,-4.2346843748,0.8060420222,0.0115621853,-2.858490084,4.6921950
828,0.0075252078,-0.6133273944,-4.572847159,0.0040636874,-5.0669499256
, -3.2032831849,0.0146338786,-6.2165919651,1.3345233616,0.0162709593,3.
2642908147,-1.1208940856,-0.0065717859,4.3030385122,-3.6647486745,-0.0
10018017,3.703116276,-4.6544049994,1.6987305874,6.3402393626,-3.397028
4551,-0.0200491338,3.6866180805,-4.6572395374,-1.7111689855\PG=C01 [X(
C7H7O1)]\NImag=0\

³p-hydroxyphenyl cation

\1,3\C,0,-2.6834472279,2.602186985,0.\C,0,-3.9265771605,1.953708977
9,0.\C,0,-1.4157157273,2.0143116634,0.\C,0,-1.3854555742,0.6409849249,
0.\C,0,-3.8993922807,0.5809525208,0.\C,0,-2.6275869341,-0.0833585719,0
.\H,0,-4.8584504751,2.5081383232,0.\H,0,-0.50836871,2.6077546034,0.\H,
0,-0.4613482819,0.0732689844,0.\H,0,-4.8135562759,-0.0056950005,0.\O,0
, -2.5189405142,-1.3856127569,0.\H,0,-3.3736808382,-1.8491806536,0.\Ve
rsion=EM64L-G09RevB.01\State=3-A"\MP2/GTBas1=-305.5013103\MP4/GTBas1=-
305.5903824\CCSD(T)/G3Bas1=-305.601278\MP2/GTBas2=-305.5126858\MP4/GTB
as2=-305.6025104\MP2/GTBas3=-305.7085974\MP4/GTBas3=-305.8092475\HF/GT
LargeXP=-304.7585398\MP2/GTLargeXP=-306.133549\HF/GFHFB1=-304.7836046\
HF/GFHFB2=-304.7883031\G4=-306.3052028\FreqCoord=-5.0709803527,4.91742
07481,0.,-7.420155473,3.6919749116,0.,-2.6753150067,3.80649739,0.,-2.6
181316046,1.2112859633,0.,-7.3687834952,1.0978411606,0.,-4.9654196958,
-0.1575248717,0.,-9.1811408282,4.7396945342,0.,-0.9606776364,4.9279420
223,0.,-0.8718219046,0.1384583145,0.,-9.0963030867,-0.0107619912,0.,-4
.7601077168,-2.6184286368,0.,-6.3753328439,-3.4944450056,0.\PG=CS [SG(
C6H5O1)]\NImag=0\

³p-thiolphenyl cation

\1,3\C,0,-2.6885709496,2.6562661799,0.\C,0,-3.9198507757,2.00610874
16,0.\C,0,-1.4257825568,2.074889088,0.\C,0,-1.3909585618,0.6957058759,
0.\C,0,-3.885123976,0.6274740376,0.\C,0,-2.6205614463,-0.0394367137,0.
\H,0,-4.858031641,2.5498461327,0.\H,0,-0.5171100431,2.6663054398,0.\H,
0,-0.4452748396,0.1626838567,0.\H,0,-4.8039928292,0.0508638019,0.\S,0,
-2.4763490209,-1.7438754129,0.\H,0,-3.7927433601,-2.0504510275,0.\Ver
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/GFHFB2=-627.440345\G4=-629.1798992\FreqCoord=-5.0806627835,5.01961561
6,0.,-7.4074444479,3.7909961144,0.,-2.6943385574,3.9209721324,0.,-2.62
8530744,1.3146935745,0.,-7.341820307,1.1857540866,0.,-4.9521434479,-0.
0745245885,0.,-9.1803493464,4.8185108719,0.,-0.9771963619,5.0385870679
,0.,-0.8414475007,0.3074279354,0.,-9.0782307915,0.0961186557,0.,-4.679
621459,-3.2954469403,0.,-7.1672462428,-3.8747908909,0.\PG=CS [SG(C6H5S
1)]\NImag=0\

³m-nitrophenyl cation

\1,3\C,0,-2.7107659461,2.9045334061,0.\C,0,-3.928793144,2.1760852
73,0.\C,0,-1.4966209152,2.2718079135,0.\C,0,-1.5789912209,0.8596837435
,0.\C,0,-3.9293824073,0.7423587872,0.\C,0,-2.7321300329,0.060734172,0.
\N,0,-2.7711910887,4.3933919312,0.\H,0,-4.859303834,2.7349930325,0.\H,
0,-4.8791419512,0.2173927281,0.\H,0,-2.6734565868,-1.0222870024,0.\H,0
, -0.5596191096,2.8194271666,0.\O,0,-1.7096787462,4.977187523,0.\O,0,-3
.8934650172,4.8730113258,0.\Version=EM64L-G09RevB.01\State=3-A"\MP2/G
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5\MP4/GTBas3=-434.8221234\HF/GTLargeXP=-433.353034\MP2/GTLargeXP=-435.2802543\HF/GFHFB1=-433.3882779\HF/GFHFB2=-433.3950172\G4=-435.5052869\FreqCoord=-5.1226052486,5.4887726813,0.,-7.4243430749,4.1122052078,0.,-2.8282036544,4.293094783,0.,-2.9838609737,1.6245668361,0.,-7.4254566212,1.4028548002,0.,-5.1629775216,0.1147709521,0.,-5.2367922196,8.3023075445,0.,-9.1827534427,5.1683878067,0.,-9.2202420512,0.4108127193,0.,-5.0521007772,-1.9318424638,0.,-1.0575268559,5.3279451965,0.,-3.2308246055,9.4055213305,0.,-7.3575825904,9.2086568481,0.\PG=CS [SG(C6H4N1O2)]\NImag=1\\

³o-nitrophenyl cation

\1,3\C,0,-2.8107432114,2.9931977336,0.\C,0,-3.9889228708,2.1740450884,0.\C,0,-1.6018084541,2.3590864449,0.\C,0,-1.5757919612,0.9570653966,0.\C,0,-3.9278300555,0.7471772426,0.\C,0,-2.7032899647,0.1133806333,0.\H,0,-2.8677963145,4.0774267076,0.\H,0,-4.9601249257,2.660551591,0.\N,0,-0.3180044186,3.087750174,0.\H,0,-4.8504510003,0.1764217995,0.\H,0,-2.601347693,-0.9668870574,0.\O,0,0.6690319506,2.3640785734,0.\O,0,-0.3627010807,4.2976556725,0.\Version=EM64L-G09RevB.01\State=3-A"\MP2/GTBas1=-434.4257793\MP4/GTBas1=-434.526517\CCSD(T)/G3Bas1=-434.5210035\MP2/GTBas2=-434.4457213\MP4/GTBas2=-434.5480498\MP2/GTBas3=-434.7010753\MP4/GTBas3=-434.8179417\HF/GTLargeXP=-433.3490173\MP2/GTLargeXP=-435.2760576\HF/GFHFB1=-433.3844432\HF/GFHFB2=-433.3911653\G4=-435.5013841\FreqCoord=-5.3115348994,5.6563239782,0.,-7.5379717911,4.1083498175,0.,-3.0269792956,4.4580273047,0.,-2.977815249,1.8085914908,0.,-7.4225231014,1.4119603613,0.,-5.1084776911,0.2142583456,0.,-5.4193496393,7.7052198042,0.,-9.3732776945,5.0277138694,0.,-0.6009412602,5.8350021956,0.,-9.1660240116,0.333388885,0.,-4.9158347162,-1.8271517399,0.,1.2642871607,4.4674610604,0.,-0.6854057106,8.1213922345,0.\PG=CS [SG(C6H4N1O2)]\NImag=1\\

³p-nitrophenyl cation

\1,3\C,0,-2.7249482826,2.8862612846,0.\C,0,-3.8921850444,2.1408493301,0.\C,0,-1.4418866546,2.1939100327,0.\C,0,-1.4700335101,0.8254996111,0.\C,0,-3.8817528462,0.7558944398,0.\C,0,-2.602391595,0.0567396335,0.\N,0,-5.1990932387,2.8505074102,0.\O,0,-5.1498930407,4.0660226912,0.\O,0,-6.1917598945,2.1472800573,0.\H,0,-2.7734363754,3.9708048957,0.\H,0,-0.5213386945,2.7705600901,0.\H,0,-4.8178076681,0.2059939195,0.\H,0,-2.5847831552,-1.0293633956,0.\Version=EM64L-G09RevB.01\State=3-A"\MP2/GTBas1=-434.4206799\MP4/GTBas1=-434.5227346\CCSD(T)/G3Bas1=-434.5167549\MP2/GTBas2=-434.4406364\MP4/GTBas2=-434.5442526\MP2/GTBas3=-434.696563\MP4/GTBas3=-434.8148365\HF/GTLargeXP=-433.3417107\MP2/GTLargeXP=-435.2717931\HF/GFHFB1=-433.3770148\HF/GFHFB2=-433.3837546\G4=-435.5002702\FreqCoord=-5.1494059803,5.4542433758,0.,-7.3551637924,4.0456189256,0.,-2.7247708919,4.1458891219,0.,-2.7779607403,1.5599681877,0.,-7.3354497949,1.4284334766,0.,-4.9178074051,0.1072223681,0.,-9.8248623605,5.3866783451,0.,-9.7318874605,7.6836693365,0.,-11.7007304812,4.0577712389,0.,-5.2410351964,7.5037337801,0.,-0.9851873551,5.2355998049,0.,-9.1043370535,0.3892720928,0.,-4.8845322763,-1.9452149089,0.\PG=CS [SG(C6H4N1O2)]\NImag=1\\

G4MP2 archive entries

¹syn-m-thiomethoxyphenyl cation

```
\1,1\C,0,-0.2703178765,1.2136560608,-0.1210086609\C,0,-1.5888
61379,1.2557567248,-0.1043311574\C,0,-2.6882012185,0.5328315004,0.0393
143575\C,0,-2.26519144,-0.8445560275,0.0404742744\C,0,-0.925199557,-1.
1709869318,0.101029552\C,0,0.0957797321,-0.1886339927,0.0417081524\H,0
,0.4246429814,1.9553717935,-0.4889568963\H,0,-3.6769681248,0.847198004
5,0.3464235964\H,0,-3.0345795723,-1.5993295066,0.1728722733\H,0,-0.637
313178,-2.210090229,0.2108836937\S,0,1.7283664688,-0.7073783442,-0.181
7823457\C,0,2.7235949245,0.7435116882,0.2659764542\H,0,2.422483414,1.1
369080333,1.2372681763\H,0,3.7497020853,0.3736027096,0.3185238678\H,0,
2.67150674,1.5083715169,-0.5131473378\\Version=EM64L-G09RevB.01\State=
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85\HF/GFHFB3=-666.4193412\HF/GFHFB4=-666.4426194\G4MP2=-667.9000537\Fr
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62993,-0.1971573146,-5.079964093,1.0069056107,0.0742933688,-4.28059146
02,-1.5959795959,0.076485294,-1.748373781,-2.2128446063,0.1909181847,0
.1809974627,-0.3564665855,0.0788169856,0.8024589391,3.6951171777,-0.92
39946248,-6.9484627553,1.6009722089,0.6546457231,-5.7345243201,-3.0222
947637,0.3266812525,-1.2043473672,-4.1764652618,0.398512427,3.26613928
32,-1.3367513429,-0.3435188492,5.1468485042,1.4050334673,0.5026226562,
4.577830214,2.1484448212,2.3380980062,7.0859100212,0.7060068036,0.6019
22877,5.0484161007,2.8504090736,-0.9697079343\PG=C01 [X(C7H7S1)]\NImag
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```

¹syn-o-thiomethoxyphenyl cation

```
\1,1\C,0,-0.5046643696,0.8702498652,-0.1190069907\C,0,-1.6913
450434,1.4577284423,-0.0203677981\C,0,-2.635205575,0.3928844641,0.0722
090241\C,0,-2.1928697702,-0.932060011,0.0820186809\C,0,-0.8481636323,-
1.2503737376,0.0052842893\C,0,0.2059303427,-0.2516850762,-0.0979212354
\H,0,-1.960203219,2.4980556142,-0.1434359115\H,0,-3.6851709998,0.66541
86011,0.0461059954\H,0,-2.91521536,-1.7355025068,0.1667183277\H,0,-0.4
866197916,-2.270221675,0.1203428656\S,0,1.8936285689,-0.6545618333,-0.
0639806631\C,0,2.6657997891,0.9870049051,0.134359282\H,0,2.4304522603,
1.4134592967,1.1095708741\H,0,3.7385493712,0.7943510389,0.0735309583\H
,0,2.3742004288,1.6496466122,-0.6833936985\\Version=EM64L-G09RevB.01\St
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6737821\HF/GFHFB3=-666.4227138\HF/GFHFB4=-666.4459593\G4MP2=-667.89230
26\FreqCoord=-0.9536774475,1.6445339124,-0.2248906202,-3.1961789283,2.
7547075321,-0.0384895604,-4.9798168406,0.742444039,0.1364552798,-4.143
9233107,-1.7613381602,0.1549928446,-1.6027969809,-2.3628639278,0.00998
58597,0.3891519501,-0.4756158658,-0.1850443175,-3.7042472488,4.7206409
756,-0.2710545903,-6.9639639425,1.2574589198,0.0871277044,-5.508958648
8,-3.2796244407,0.3150519807,-0.919578137,-4.2900972266,0.227415058,3.
5784393926,-1.236942602,-0.1209059311,5.0376315265,1.8651689624,0.2539
022464,4.592889151,2.6710509708,2.096785077,7.0648344459,1.501105917,0
.1389533735,4.4865885949,3.1173803131,-1.2914269312\PG=C01 [X(C7H7S1)]
\NImag=0\\
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¹syn-m-methoxyphenyl cation

```
\1,1\C,0,1.2388739653,-1.2117427224,-0.0186943332\C,0,-0.0802
180973,-1.1532263875,-0.0491054784\C,0,-0.4409603319,0.2550351087,0.01
41059292\C,0,0.595700528,1.2227442485,-0.0078035276\C,0,1.9197408959,0
.8521822126,-0.0238216376\C,0,2.3628214662,-0.5317958561,0.0405718955\
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H,0,-0.773610901,-1.9032537786,-0.4076041595\H,0,0.3153639999,2.268429
2668,0.0102839579\H,0,2.706069896,1.592573585,0.0977744835\H,0,3.35694
7686,-0.8184835805,0.3514997502\O,0,-1.6794094484,0.6568228058,-0.1123
334112\C,0,-2.7811768272,-0.2445333921,0.1218362959\H,0,-2.624652815,-
0.8029074681,1.0481653976\H,0,-3.6607699515,0.3916819795,0.2015736355\
H,0,-2.8934090649,-0.9191500217,-0.7328717977\\Version=EM64L-G09RevB.0
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45.0686051\HF/GFHFB3=-343.7548103\HF/GFHFB4=-343.7798429\G4MP2=-345.27
118\FreqCoord=2.3411325075,-2.2898618888,-0.03532717,-0.1515902349,-2.
1792820416,-0.0927959058,-0.8332942627,0.4819465097,0.026656343,1.1257
108551,2.3106517603,-0.01474653,3.6277845394,1.6103909971,-0.045016371
,4.465085472,-1.0049485267,0.0766697711,-1.4619127364,-3.5966284029,-0
.770260232,0.595951592,4.286710066,0.0194338639,5.1137309998,3.0095279
222,0.1847669966,6.3437117689,-1.5467098114,0.6642382636,-3.1736239225
,1.2412152208,-0.2122793827,-5.2556625306,-0.4621011414,0.2302372323,-
4.9598750143,-1.5172752247,1.9807455434,-6.9178526438,0.7401716724,0.3
809189666,-5.467750723,-1.7369418161,-1.3849269882\PG=C01 [X(C7H7O1)]\
NImag=0\\

¹syn-o-methoxyphenyl cation

\\1,1\C,0,-1.3496507949,1.4112771453,0.0158660867\C,0,-0.13336
41303,0.8842959891,-0.0588592095\C,0,0.5700651976,-0.261467636,-0.1445
408891\C,0,-0.4845836408,-1.2462334032,-0.0368105578\C,0,-1.8382120363
, -0.9590201907,0.0576979656\C,0,-2.3029498504,0.3527041968,0.106228190
6\H,0,-1.6303088888,2.4380330795,-0.1897675663\H,0,-0.0847238165,-2.24
07260603,0.1628763873\H,0,-2.5397257154,-1.7828125018,0.1247611747\H,0
, -3.3541598742,0.6153535667,0.0640920245\O,0,1.829624787,-0.5904390136
, -0.1365322415\C,0,2.7808143738,0.4641899067,0.1642861894\H,0,2.716281
1628,0.7266444326,1.2225469017\H,0,3.7596273275,0.051896703,-0.0698169
636\H,0,2.5695178991,1.332750786,-0.4711854926\\Version=EM64L-G09RevB.
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1.6710772397,-0.1112277864,1.0772671014,-0.4941022246,-0.2731426953,-0
.9157303696,-2.3550398296,-0.0695618731,-3.4737173229,-1.8122855164,0.
1090333533,-4.351944515,0.6665143378,0.2007421878,-3.0808373119,4.6072
148232,-0.3586087292,-0.1601048101,-4.2343585929,0.3077917655,-4.79938
60548,-3.3690273746,0.2357644522,-6.3384435681,1.1628497159,0.12111637
35,3.4574897733,-1.1157680339,-0.2580085447,5.2549775929,0.8771917972,
0.3104559054,5.1330274975,1.3731589737,2.3102788287,7.1046660106,0.098
0705559,-0.1319349407,4.8556851229,2.5185339889,-0.8904115387\PG=C01 [X
(C7H7O1)]\NImag=0\\

¹anti-m-thiomethoxyphenyl cation

\\1,1\C,0,-3.5279323536,3.6141388216,0.2165152389\C,0,-4.7124
064702,2.9557743923,-0.0571486728\C,0,-2.2883730699,2.9380702829,0.284
8509056\C,0,-4.7645669376,1.520985275,-0.1785143756\C,0,-3.5058041501,
1.114494167,-0.1455418325\C,0,-2.2547026348,1.499913423,0.0177416266\H
,0,-5.67509856,0.9530684105,-0.0421286856\S,0,-0.7337306188,3.68040808
73,0.4273862788\H,0,-3.559542569,4.6794208161,0.4042375829\H,0,-5.6654
854897,3.4740748945,-0.0016570766\C,0,-0.9883244209,5.4054459521,-0.09
72141396\H,0,0.0167699175,5.830260934,-0.134593513\H,0,-1.58430279,5.9
531441692,0.6337321722\H,0,-1.4362730908,5.4407218415,-1.0910013909\H,
0,-1.3461567621,0.9851185332,-0.2619141186\\Version=EM64L-G09RevB.01\St
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¹anti-o-thiomethoxyphenyl cation

\1,1\C,0,-3.4992199216,3.6064392283,-0.0008174707\C,0,-4.707624665,2.9242740382,-0.0004417656\C,0,-2.1961459093,2.9596243628,-0.0019297461\C,0,-4.7631747504,1.5316445136,-0.0010966216\C,0,-3.5483733264,0.7846960274,-0.0021315737\C,0,-2.5788397035,1.6882666641,-0.0015031015\H,0,-5.6908457268,0.9698934717,0.000660632\S,0,-0.6088696546,3.6799300313,-0.0057279607\H,0,-3.4591316596,4.6917418727,-0.002202989\H,0,-5.6268254876,3.498071948,0.0000013614\C,0,-0.9850207681,5.4586448015,-0.0031566873\H,0,0.0019160501,5.9275887237,-0.0043373618\H,0,-1.5152268666,5.7513035735,0.9040770115\H,0,-1.5182784137,5.7532155829,-0.9079929082\H,0,-3.486059197,-0.2949748398,-0.0009408187\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-667.2951367\CCSD(T)/GTBas1=-667.3992662\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-666.4158365\MP2/GTMP2LargeXP=-667.6743586\HF/GFHFB3=-666.4233763\HF/GFHFB4=-666.4466258\G4MP2=-667.8925204\FreqCoord=-6.6125673305,6.8151824564,-0.0015447957,-8.8961213532,5.5260770697,-0.0008348159,-4.1501143165,5.5928795019,-0.0036466916,-9.0010958013,2.8943886637,-0.0020723145,-6.7054538042,1.4828605894,-0.0040280905,-4.8733007801,3.1903616344,-0.0028404502,-10.7541398882,1.8328330397,0.0012484136,-1.1505968978,6.9540599473,-0.010824277,-6.5368114942,8.8661072257,-0.0041630459,-10.633159169,6.6103979748,0.000025726,-1.8614194869,10.3153437316,-0.0059652745,0.0036208099,11.2015193162,-0.0081964259,-2.8633638071,10.8683886609,1.7084579547,-2.8691303953,10.8720018352,-1.7158579272,-6.5876971654,-0.5574216633,-0.0017778897\PG=C01 [X(C7H7S1)]\NImag=0\

¹anti-m-methoxyphenyl cation

\1,1\C,0,-3.5424455642,3.7492821724,0.0709901292\C,0,-4.673761527,2.9757496893,-0.100059086\C,0,-2.2625617554,3.1572779772,0.1930902871\C,0,-4.6704555401,1.5271561672,-0.1310249394\C,0,-3.3875755101,1.2369637075,-0.0465195089\C,0,-2.1622570246,1.7099590077,0.0561433617\H,0,-5.5528959273,0.9338837761,0.0591578958\O,0,-1.1138025783,3.7774894161,0.2573565166\H,0,-3.6484967782,4.8227108194,0.1524508208\H,0,-5.6613268193,3.4240072264,-0.0222780266\C,0,-1.0290590854,5.1961635202,-0.0286440493\H,0,0.036059255,5.4166935186,-0.0494604496\H,0,-1.5152456143,5.7619660885,0.7698686117\H,0,-1.4846724729,5.4114044941,-0.9981056099\H,0,-1.2208730578,1.2457124193,-0.2082359532\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-344.6903398\CCSD(T)/GTBas1=-344.7849274\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-343.7518832\MP2/GTMP2LargeXP=-345.0683321\HF/GFHFB3=-343.7552177\HF/GFHFB4=-343.7802361\G4MP2=-345.2703935\FreqCoord=-6.694251957,7.0851165007,0.1341519024,-8.8321292965,5.6233519528,-0.1890842696,-4.2756220765,5.9663907023,0.3648877616,-8.8258818866,2.8859069182,-0.2476012521,-6.4015899686,2.3375226434,-0.0879091316,-4.0860736054,3.231354223,0.1060955778,-10.4934525469,1.7647845769,0.1117922216,-2.1047818391,7.1384204663,0.4863333348,-6.894659

7076,9.1136026668,0.2880903001,-10.6983572373,6.470435935,-0.042099369
,-1.9446398459,9.8193259948,-0.0541294085,0.0681421166,10.2360672959,-
0.0934667042,-2.8633992351,10.8885378942,1.4548408344,-2.8056243707,10
.2260724881,-1.8861462544,-2.3071157223,2.3540553128,-0.3935089226\PG=
C01 [X(C7H7O1)]\NImag=0\

¹anti-o-methoxyphenyl cation

\1,1\C,0,-3.5293817276,3.7140423176,-0.0034641923\C,0,-4.691
4133754,2.9530086807,-0.0023388108\C,0,-2.192245919,3.1725231001,-0.00
1854027\C,0,-4.6553987639,1.5623079674,0.0010076461\C,0,-3.3897090875,
0.9048733613,0.0031672846\C,0,-2.4656724508,1.8529015151,0.0013049187\
H,0,-5.5400004353,0.9354731291,-0.0002118721\H,0,-3.2578485097,-0.1697
823395,0.0022908778\O,0,-1.0404354545,3.7919322964,-0.0002991954\H,0,-
3.560562366,4.8014728418,-0.0022852247\H,0,-5.6463730642,3.4650761188,
-0.0037208943\C,0,-1.0118176217,5.240040026,-0.0044492364\H,0,0.047076
3254,5.4905322595,-0.0040993006\H,0,-1.4911265096,5.6297557601,0.89714
26807\H,0,-1.4894510401,5.6245629657,-0.9091406544\Version=EM64L-G09R
evB.01\State=1-A\MP2/GTBas1=-344.6721077\CCSD(T)/GTBas1=-344.7676939\M
P2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-343.7431715\MP2/GTMP2Large
XP=-345.051469\HF/GFHFB3=-343.7467435\HF/GFHFB4=-343.7717539\G4MP2=-34
5.2562328\FreqCoord=-6.6695648835,7.0185228261,-0.0065463747,-8.865486
4557,5.5803776745,-0.0044197119,-4.1427444029,5.9951998093,-0.00350360
34,-8.7974287031,2.9523341935,0.0019041752,-6.4056218456,1.7099628378,
0.0059853005,-4.6594456654,3.5014764148,0.002465939,-10.4690835988,1.7
677880186,-0.0004003802,-6.1564414658,-0.3208421238,0.0043291317,-1.96
61380679,7.1657135547,-0.0005653974,-6.7284877508,9.0734687054,-0.0043
184488,-10.6700987355,6.5480448942,-0.0070314712,-1.9120582015,9.90224
05744,-0.0084078382,0.0889613623,10.3756022942,-0.0077465556,-2.817820
7326,10.6386965817,1.6953539687,-2.8146545541,10.6288836224,-1.7180268
531\PG=C01 [X(C7H7O1)]\NImag=1\

³syn-m-thiomethoxyphenyl cation

\1,3\C,0,0.3075302504,1.2114394396,0.0000221904\C,0,1.6467
976482,1.4270000391,0.0001038764\C,0,2.6510366872,0.4644922094,0.00011
39566\C,0,2.2477750728,-0.8846594831,0.0000048338\C,0,0.9020671516,-1.
194450014,-0.0000864373\C,0,-0.087046425,-0.1581285315,-0.0000762197\H
,0,-0.4138930038,2.0184436445,-0.000016554\H,0,3.7017488917,0.73542504
15,0.0001930725\H,0,2.9904122817,-1.6744383463,-0.0000037942\H,0,0.579
3404108,-2.2302336047,-0.0001746545\S,0,-1.7049756354,-0.7206126683,-0
.0002299349\C,0,-2.7661826184,0.7461483559,0.000108013\H,0,-2.59316972
38,1.3370944828,-0.901645403\H,0,-3.7862647723,0.3586019594,-0.0008349
811\H,0,-2.5943882159,1.3358674757,0.9028910207\Version=EM64L-G09RevB
.01\State=3-A\MP2/GTBas1=-667.2873088\CCSD(T)/GTBas1=-667.4073003\MP2/
GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-666.4549376\MP2/GTMP2LargeXP=
-667.6595742\HF/GFHFB3=-666.4619855\HF/GFHFB4=-666.4853947\G4MP2=-667.
8935574\FreqCoord=0.5811479509,2.2892887674,0.0000419337,3.1119965514,
2.6966392655,0.0001962979,5.009733307,0.8777630665,0.0002153468,4.2476
792959,-1.6717641439,0.0000091346,1.7046598701,-2.257183406,-0.0001633
429,-0.1644939041,-0.2988196183,-0.0001440344,-0.7821444255,3.81430570
28,-0.0000312825,6.995291618,1.3897519197,0.0003648542,5.6510602369,-3
.1642299009,-0.00000717,1.094794714,-4.2145307253,-0.0003300493,-3.221
9370141,-1.361760591,-0.0004345139,-5.2273275823,1.4100160472,0.000204
115,-4.900380594,2.5267423863,-1.7038628806,-7.1550034862,0.677659494,
-0.0015778857,-4.9026832104,2.524423679,1.706216757\PG=C01 [X(C7H7S1)]
\NImag=0\

³syn-o-thiomethoxyphenyl cation

\\1,3\C,0,0.8345047317,-1.2864220919,0.0000123339\C,0,-0.14
4356751,-0.238942352,0.0000671438\C,0,0.3301072595,1.0785482291,0.0001
348146\C,0,1.6372819608,1.4508807519,0.0001502544\C,0,2.5802651046,0.3
97883163,0.0000992712\C,0,2.1690533194,-0.9524126298,0.0000285945\H,0,
0.511132607,-2.3223986486,-0.0000437328\H,0,1.9551470203,2.4874514809,
0.000197374\H,0,3.6391504199,0.6364869313,0.0001089865\H,0,2.918506533
1,-1.7351145894,-0.0000141067\S,0,-1.7944293416,-0.673330563,0.0000295
561\C,0,-2.6918101192,0.9025379238,0.0001495506\H,0,-2.440833381,1.467
0880997,-0.8995160431\H,0,-3.7495033318,0.6355699826,-0.0000829776\H,0
, -2.4411610317,1.4667143127,0.9001469807\\Version=EM64L-G09RevB.01\Sta
te=3-A\MP2/GTBas1=-667.276298\CCSD(T)/GTBas1=-667.4108577\MP2/GTBas2=0
.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-666.471068\MP2/GTMP2LargeXP=-667.6471
08\HF/GFHFB3=-666.4781456\HF/GFHFB4=-666.5015256\G4MP2=-667.8958017\Fr
eqCoord=1.5769853995,-2.430985445,0.0000233077,-0.2727947249,-0.451535
6069,0.0001268835,0.6238123149,2.0381607741,0.0002547626,3.0940145082,
2.7417672725,0.0002839396,4.875994398,0.7518902109,0.0001875953,4.0989
167413,-1.7997990359,0.0000540358,0.9659006449,-4.3886974173,-0.000082
643,3.6946924179,4.7006020678,0.0003729828,6.87699765,1.2027859873,0.0
002059547,5.5151780646,-3.278891383,-0.0000266579,-3.3909800204,-1.272
410361,0.0000558529,-5.086783927,1.7055495004,0.0002826096,-4.61250662
62,2.7723947212,-1.6998389737,-7.0855344314,1.2010532054,-0.000156805,
-4.6131257962,2.7716883661,1.7010312729\PG=C01 [X(C7H7S1)]\NImag=0\\

³syn-m-methoxyphenyl cation

\\1,3\C,0,-1.2704218276,1.4026830375,0.0000255209\C,0,0.0599
309301,1.1720673711,0.0000249552\C,0,0.4238038553,-0.2128437795,-0.000
0027432\C,0,-0.5929251056,-1.2414738177,-0.0000208332\C,0,-1.926874839
8,-0.9103458421,-0.0000218542\C,0,-2.3027417038,0.4508867037,0.0000070
044\H,0,0.8010368747,1.9615609077,0.0000520437\H,0,-0.2529041908,-2.27
05527983,-0.0000400679\H,0,-2.6871476092,-1.6830024939,-0.0000427722\H
,0,-3.3464724642,0.7476504653,-0.0000000214\O,0,1.6445206657,-0.664249
7762,-0.0000099716\C,0,2.797942928,0.2203226727,-0.0000414702\H,0,2.78
4235361,0.8354678446,0.9022524242\H,0,3.6588918218,-0.4438924346,-0.00
02059901\H,0,2.7840503043,0.8356799398,-0.9021862244\\Version=EM64L-G0
9RevB.01\State=3-A\MP2/GTBas1=-344.6686239\CCSD(T)/GTBas1=-344.778605\
MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-343.7892523\MP2/GTMP2Larg
eXP=-345.0397551\HF/GFHFB3=-343.7924452\HF/GFHFB4=-343.8174548\G4MP2=-
345.2583627\FreqCoord=-2.4007493274,2.650686792,0.0000482275,0.1132530
448,2.2148863407,0.0000471585,0.8008732206,-0.4022164523,-0.000005184,
-1.120466067,-2.3460455167,-0.000039369,-3.6412657395,-1.7203043277,-0
.0000412985,-4.3515511749,0.8520523869,0.0000132365,1.5137403156,3.706
8129085,0.0000983483,-0.4779196584,-4.290722959,-0.0000757174,-5.07797
30601,-3.1804137944,-0.0000808278,-6.3239164685,1.4128546225,-0.000000
0404,3.1076936781,-1.2552501609,-0.0000188436,5.2873458693,0.416349512
2,-0.0000783673,5.2614423219,1.5788054191,1.7050099845,6.914303493,-0.
8388351339,-0.0003892649,5.2610926152,1.5792062209,-1.704884885\PG=C01
[X(C7H7O1)]\NImag=0\\

³syn-o-methoxyphenyl cation

\\1,3\C,0,-1.2888139833,1.4275274467,-0.0006786727\C,0,0.014
8128486,1.0672088517,-0.0012472669\C,0,0.4883194497,-0.27119726,-0.000
8103408\C,0,-0.4941928464,-1.3242836077,0.0003625948\C,0,-1.8215014662
, -0.9919420537,0.000964146\C,0,-2.2359320288,0.367626256,0.0005215453\
H,0,-1.6139010831,2.4624731529,-0.0004620114\H,0,-0.140613594,-2.34949
65387,0.0004437735\H,0,-2.5748882408,-1.7710246897,0.00169012\H,0,-3.2
950026002,0.6056262458,0.0014821169\O,0,1.73601705,-0.6150007574,-0.00

18342466\C,0,2.7846205378,0.3997366476,0.0020718807\H,0,2.7326534484,0.9560794419,0.9401392763\H,0,3.7148625762,-0.1581821155,-0.0717709384\H,0,2.6489839322,1.0601719799,-0.8564139768\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-344.6602029\CCSD(T)/GTBas1=-344.7804869\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-343.7988845\MP2/GTMP2LargeXP=-345.0296432\HF/GFHFB3=-343.802122\HF/GFHFB4=-343.8271326\G4MP2=-345.2588337\FreqCoord=-2.4355054647,2.6976359214,-0.0012825055,0.0279922271,2.0167324563,-0.0023569929,0.9227900253,-0.5124885494,-0.0015313222,-0.9338891365,-2.5025333408,0.0006852049,-3.4421389218,-1.8744988212,0.0018219719,-4.2252991862,0.6947129431,0.0009855778,-3.0498310526,4.6533998686,-0.000873075,-0.2657211832,-4.4399050083,0.0008386104,-4.8658335979,-3.3467516381,0.0031938639,-6.2266525215,1.1444677434,0.002800795,3.2805967865,-1.162183003,-0.0034662237,5.2621702005,0.7553927892,0.0039152871,5.1639666336,1.8067283065,1.776605759,7.0200728903,-0.2989208774,-0.1356274179,5.0058541623,2.0034346958,-1.6183878725\PG=C01 [X(C7H7O1)]\NImag=1\\

³anti-m-thiomethoxyphenyl cation

\\1,3\C,0,-3.5245933647,3.6377126389,-0.0029846047\C,0,-4.7223158176,2.9543900364,-0.0025010073\C,0,-2.2926162422,2.9245455337,-0.0003682009\C,0,-4.7346410812,1.5390104491,0.0006005231\C,0,-3.5085137164,0.8956338201,0.0030605252\C,0,-2.2888972292,1.4885017133,0.002795552\H,0,-5.671636113,0.9917414591,0.0010075156\S,0,-0.7407446154,3.6485894008,-0.0006356875\H,0,-3.5256598893,4.7197959337,-0.0053652736\H,0,-5.6599324293,3.4991561785,-0.0044976018\C,0,-0.9864156486,5.4431423418,-0.0047188528\H,0,0.0204521282,5.8642279452,-0.0048092809\H,0,-1.517913466,5.7544000697,0.8966103249\H,0,-1.5164394425,5.7504931396,-0.9082547174\H,0,-1.356063073,0.9336993401,0.0048107862\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-667.2831313\CCSD(T)/GTBas1=-667.4060508\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-666.4533769\MP2/GTMP2LargeXP=-667.6560197\HF/GFHFB3=-666.4603929\HF/GFHFB4=-666.4838309\G4MP2=-667.8930393\FreqCoord=-6.6605161891,6.8742806376,-0.0056400856,-8.9238836082,5.5829880585,-0.0047262188,-4.3324168257,5.5265901219,-0.0006957989,-8.9471749809,2.9083082644,0.0011348241,-6.6301300575,1.6925026353,0.0057835545,-4.3253889095,2.8128605865,0.0052828276,-10.7178389789,1.8741197522,0.0019039286,-1.3998044575,6.8948347389,-0.0012012753,-6.6625316285,8.9191217178,-0.0101388977,-10.6957222219,6.6124468736,-0.0084992357,-1.864055429,10.2860483283,-0.0089173395,0.0386489212,11.0817847973,-0.0090882238,-2.8684407441,10.8742401908,1.6943479619,-2.8656552434,10.8668571629,-1.7163526748,-2.5625878268,1.7644360433,0.0090910684\PG=C01 [X(C7H7S1)]\NImag=0\\

³anti-o-thiomethoxyphenyl cation

\\1,3\C,0,-3.5477953793,3.6750796509,-0.0034311039\C,0,-4.7187132238,2.952056643,-0.0026910188\C,0,-2.3064951786,2.9714644719,-0.0011453671\C,0,-4.713855259,1.5359066276,0.0002850845\C,0,-3.5062513484,0.8129535429,0.0026198434\C,0,-2.3720162039,1.5653348355,0.0017957082\H,0,-5.6572123931,0.9990422126,0.0007856925\S,0,-0.737201247,3.6454202419,-0.0014814793\H,0,-3.5676199483,4.7579160706,-0.0056984754\H,0,-5.6688337742,3.473874406,-0.0044058901\C,0,-0.9612927308,5.4428021857,-0.0043573901\H,0,0.0494155571,5.8543458513,-0.0048183691\H,0,-1.4900653361,5.7589927815,0.8970580236\H,0,-1.4897367914,5.7561365047,-0.9069621451\H,0,-3.4940467433,-0.2709660261,0.0049068868\\Version=EM64L-G09RevB.01\State=3-A\MP2/GTBas1=-667.274637\CCSD(T)/GTBas1=-667.4086831\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-666.4685772\MP2/GTMP2LargeXP=-667.6456378\HF/GFHFB3=-666.4756624\HF/GFHFB4=-666.4990416\G4MP2=-667.893605\FreqCoord=-6.7043616423,6.9448940568,-0.0064838466,-8.917075

6927,5.5785785841,-0.0050852886,-4.3586442144,5.6152540654,-0.00216443
02,-8.9078954696,2.9024428918,0.0005387316,-6.6258548015,1.5362595549,
0.0049507866,-4.4824610081,2.9580541454,0.0033933968,-10.6905820984,1.
8879161769,0.0014847436,-1.3931084617,6.8888458964,-0.0027995902,-6.74
18246486,8.9911583367,-0.0107685578,-10.7125433261,6.5646712475,-0.008
3259256,-1.8165799947,10.2854055264,-0.008234274,0.0933818696,11.06311
03461,-0.0091053981,-2.8158154053,10.8829191584,1.69519399,-2.81519454
58,10.8775215774,-1.7139100672,-6.6027914403,-0.5120515806,0.009272672
2\PG=C01 [X(C7H7S1)]\NImag=0\

³anti-m-methoxyphenyl cation

\1,3\C,0,-3.5650333706,3.769809059,-0.0030057741\C,0,-4.70
54211846,3.0082125029,-0.0023379602\C,0,-2.2778506353,3.1289110669,-0.
000827769\C,0,-4.621183193,1.5856182806,0.0004953996\C,0,-3.3470348886
,1.019581378,0.002537816\C,0,-2.1762051238,1.6876427898,0.0020858163\H
,0,-5.5200395581,0.9774706197,0.0010215711\O,0,-1.1422971079,3.7610290
78,-0.0012401574\H,0,-3.6274615464,4.8501023806,-0.0051258539\H,0,-5.6
806733902,3.4824375022,-0.0039533585\C,0,-1.0414175168,5.2117145303,-0
.0041672422\H,0,0.0270535427,5.4140765335,-0.0043179009\H,0,-1.5093682
941,5.6123128015,0.8974152713\H,0,-1.5089466457,5.6087125254,-0.907552
3583\H,0,-1.1934910876,1.2287889515,0.0037025002\Version=EM64L-G09Rev
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.256446\FreqCoord=-6.736936725,7.1239066947,-0.0056800898,-8.891957378
8,5.6846977799,-0.0044181045,-4.3045138722,5.9127850107,-0.0015642568,
-8.7327706446,2.9963843017,0.0009361696,-6.3249792967,1.9267295746,0.0
047957772,-4.112431693,3.1891826828,0.0039416217,-10.4313630074,1.8471
517742,0.0019304895,-2.1586286964,7.1073149352,-0.0023435578,-6.854908
8802,9.1653652158,-0.00968646,-10.7349169578,6.5808531541,-0.007470765
, -1.9679938968,9.8487131451,-0.0078749465,0.0511237866,10.2311219108,-
0.0081596501,-2.8522927095,10.605734167,1.6958690902,-2.8514959095,10.
5989306312,-1.7150254084,-2.2553712977,2.3220745935,0.0069967113\PG=C0
1 [X(C7H7O1)]\NImag=0\

³anti-o-methoxyphenyl cation

\1,3\C,0,-3.5668724072,3.7928282423,-0.0030029233\C,0,-4.6
845002361,3.0000999717,-0.0023215582\C,0,-2.2811344079,3.160475692,-0.
0011926388\C,0,-4.5957310058,1.5750723409,0.0001190412\C,0,-3.34417995
62,0.9239205689,0.0019657659\C,0,-2.2565058049,1.7342516584,0.00125155
98\H,0,-5.507797127,0.9866058259,0.000561329\H,0,-3.2706467593,-0.1580
029603,0.0038340914\O,0,-1.1329486188,3.7651164554,-0.0015335938\H,0,-
3.6470413417,4.8726889885,-0.0048134647\H,0,-5.6669445487,3.4586361986
, -0.0036469333\C,0,-1.0236352305,5.2150420947,-0.0041150833\H,0,0.0457
731694,5.4116033703,-0.0045641983\H,0,-1.4909986463,5.616739448,0.8974
799933\H,0,-1.4911970792,5.6136421047,-0.906971387\Version=EM64L-G09R
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157,5.6693673177,-0.0043871091,-4.3107193033,5.9724335075,-0.002253760
7,-8.6846729813,2.9764553639,0.0002249552,-6.3195842563,1.7459568437,0
.0037147592,-4.2641779885,3.2772606799,0.0023651053,-10.4082281654,1.8
64414812,0.0010607582,-6.1806266524,-0.2985823232,0.0072453827,-2.1409
626122,7.1150389591,-0.0028980723,-6.8919093311,9.208047719,-0.0090961
301,-10.7089732073,6.5358752086,-0.0068917051,-1.9343902456,9.85500133
05,-0.0077763804,0.0864987544,10.2264483097,-0.0086250849,-2.817579106

,10.6140993165,1.695991397,-2.8179540898,10.608246186,-1.7139275318\PG
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