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Comment on "Activation of methane to CH_3^+: A selective industrial route to methanesulfonic acid"

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Computational Procedures, Structures, and Energies 1
General 1
Energies 2
Table 1. CCSD(T)/SMD//M06-2X Energies. 2
CAS Energies 3
M06-2X/6-31+G** Gas-Phase Structures and Energies 3
CH_3^+ 3
SO_3 3
H_2SO_4 3
CH_3–$S(O)_2O^+$ (3-*C_3V*) 3
CH_3–$S(O)_2O^+$ (3-*C_S*) 4
CH_3–$S(O)_2O^+$ (3-*open shell*) 4
$MeOSO_3H_2^+$ (4) 4
$MeOSO_2^+$ (5) 4
MSA 5
Methane 5
CH_3• (methyl radical) 5
Complex of CH_3• with SO_3 5
TS for addition of CH_3• to SO_3 (6) 5
methanesulfinicacid (CH_3OSO_2H) 5
methanesulfonyl radical (CH_3SO_3•) 6
TS for H-Atom abstraction from methane by CH_3SO_3• 6
References 7

Computational Procedures, Structures, and Energies

General

The calculations of structures, energies, and frequencies employed either Gaussian16[1] or ORCA.[2] Default procedures were employed unless otherwise noted. Complete structures and energetics are provided in sections below. All absolute energies are in Hartrees. All relative energies are presented in kcal/mol.

SMD calculations for sulfuric acid were carried out the parameters eps=109,

epsinf=2.016, and rsolv=2.5, taken from Koleva, G.; Galabov, B.; Hadjieva, B.; Schaefer, H. F.; Schleyer, P. v. R. *Angew. Chem. Int. Ed.* **54**, 14123-14127 (2015).

Energies

Table 1. CCSD(T)/SMD//M06-2X Energies.

Structure	M06-2X 6-31+G** potential energy[a]	Raw Free Energy (1 atm, 25 °C)[b]	Corrected Free Energy (1 M, 25 °C)[c]	Potential energy with SMD solvent correction[d]	CCSD(T) aug-cc-pVTZ potential energy[e]	Free energy with CCSD(T) and SMD corrections[f]	E_{rel} (kcal/mol)
CH_3^+	-39.455204	-39.440776	-39.437756	-39.591488	-39.405707	-39.524543	
SO_3	-623.644336	-623.656705	-623.653685	-623.652346	-623.088329	-623.105688	
H_2SO_4	-700.079446	-700.069117	-700.066097	-700.097390	-699.463076	-699.467671	
$CH_3–S(O)_2O^+$ (**3**-*C_3V*)	-663.014291	-662.994899	-662.990842	-663.119472	-662.450312	-662.532044	**61.6**[g]
$CH_3–S(O)_2O^+$ (**3**-*C_S*)	-663.090259	-663.069062	-663.066042	-663.199703	-662.485050	-662.570277	**37.6**[g]
$CH_3–S(O)_2O^+$ (**3**-*open shell*)	-663.057807	-663.040170	-663.037150	-663.166251	-662.444718	-662.532505	**61.3**[g]
$MeOSO_3H_2^+$ (**4**)	-739.657035	-739.609815	-739.606795	-739.756717	-738.989744	-739.039185	**-29.5**[h]
$MeOSO_2^+$ (**5**)	-663.180387	-663.159106	-663.156086	-663.282088	-662.575151	-662.652552	**-14.0**[g]
MSA	-664.180266	-664.146901	-664.143881	-664.199369	-663.567534	-663.550252	**-20.7**[j]
Methane	-40.487944	-40.460096	-40.457076	-40.489419	-40.440928	-40.411535	
CH_3• (methyl radical)	-39.811897	-39.800790	-39.797770	-39.812427	-39.763660	-39.750063	
Complex of CH_3• with SO_3	-663.470651	-663.454846	-663.451826	-663.486249	-662.862234	-662.859007	**-2.0**[i]
TS for addition of CH_3• to SO_3 (**6**)	-663.469398	-663.451428	-663.448408	-663.488078	-662.859697	-662.857388	**-1.0**[i]
methanesulfinicacid (CH_3OSO_2H)	-664.184005	-664.151757	-664.148737	-664.196899	-663.559684	-663.537310	**-12.6**[j]
methanesulfonyl radical (CH_3SO_3•)	-663.494213	-663.474227	-663.471207	-663.510414	-662.881817	-662.875014	**-12.1**[i]
TS for H-Atom abstraction from methane by CH_3SO_3•	-703.969187	-703.910475	-703.907455	-703.986866	-703.305285	-703.261233	**3.8**[k]

[a]Structures were optimized in (U)M06-2X/6-31+G** gas-phase calculations. [b]Raw free energies basic on the harmonic frequencies at 25 °C and with a 1 atm concentration. [c]Free energies corrected to 1 M. [d]Potential energies in single-point calculations including an SMD solvent correction, as described above. [e]Single-point CCSD(T)/aug-cc-pVTZ potential energies calculated using default parameters in Gaussian16. [f]Calculated as Column 4 – Column 2 + Column 5 – Column 2 + Column 6. [g]Relative to CH_3^+ and SO_3. [h]Relative to CH_3^+ and H_2SO_4. [i]Relative to CH_3• and SO_3. [j]Relative to CH_4 and SO_3. [k]Relative to CH_3•, SO_3, and methane.

CAS Energies

CAS(10,10)-NEVPT2 calculations were carried out for **3**-*open shell* and **3**-C_s in ORCA in two ways, finding the potential energies shows:

Using the options "CASNEVPT2(10,10)/aug-cc-pVDZ, TIGHTSCF"

CH_3–$S(O)_2O^+$ (**3**-*open shell*) -662.0224763

CH_3–$S(O)_2O^+$ (**3**-C_S) -662.0868931

Preference for **3**-C_S 40.4 kcal/mol.

Using the options "CASNEVPT2(10,10)/aug-cc-pVTZ + RIJCOSX def2/jk, TIGHTSCF"

CH_3–$S(O)_2O^+$ (**3**-*open shell*) -662.3312576

CH_3–$S(O)_2O^+$ (**3**-C_S) -662.3738599

Preference for **3**-C_S 26.7 kcal/mol. The 25.1 value in the main text includes the M06-2X free-energy correction and the SMD solvent model correction based on values in Table 1.

M06-2X/6-31+G** Gas-Phase Structures and Energies

The columns below provide the structures referred to in the main text, along with several closely related structures. Higher-energy conformers and a series of more tangential structures were not included.

CH_3^+

E(RM062X) = -39.4552042835

Zero-point correction= 0.031822 (Hartree/Particle)
Thermal correction to Energy= 0.034673
Thermal correction to Enthalpy= 0.035617
Thermal correction to Gibbs Free Energy= 0.014428
Sum of electronic and ZPE= -39.423383
Sum of electronic and thermal Energies= -39.420531
Sum of electronic and thermal Enthalpies= -39.419587
Sum of electronic and thermal Free Energies= -39.440776

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	21.758	6.238	44.596

H,0,0.,0.,0.0076881447
C,0,0.,0.,1.1
H,0,0.9459698156,0.,1.6461559277
H,0,-0.9459698156,0.,1.6461559277

SO_3

E(RM062X) = -623.644336054

Zero-point correction= 0.012351 (Hartree/Particle)
Thermal correction to Energy= 0.015888
Thermal correction to Enthalpy= 0.016832
Thermal correction to Gibbs Free Energy= -0.012369
Sum of electronic and ZPE= -623.631986
Sum of electronic and thermal Energies= -623.628448
Sum of electronic and thermal Enthalpies= -623.627504
Sum of electronic and thermal Free Energies= -623.656705

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	9.970	10.179	61.458

O,0,0.,0.,-0.1370178589
S,0,0.,0.,1.3
O,0,1.2444939715,0.,2.0185089294
O,0,-1.2444939715,0.,2.0185089294

H_2SO_4

E(RM062X) = -700.079446359

Zero-point correction= 0.039036 (Hartree/Particle)
Thermal correction to Energy= 0.044414
Thermal correction to Enthalpy= 0.045358
Thermal correction to Gibbs Free Energy= 0.010330
Sum of electronic and ZPE= -700.040410
Sum of electronic and thermal Energies= -700.035032
Sum of electronic and thermal Enthalpies= -700.034088
Sum of electronic and thermal Free Energies= -700.069117

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	27.870	17.979	73.724

O,0,-0.7099868458,1.289598291,-0.5937394024
S,0,-0.6000956358,1.133185134,-2.0111458616
O,0,-1.4659302413,2.3030448578,-2.6550177172
O,0,0.6723678248,1.0282958753,-2.6861882494
O,0,-1.4929804834,-0.1172253506,-2.4952880434
H,0,-1.3286762199,2.3320673026,-3.6161656446
H,0,-0.8979593986,-0.8548311102,-2.7071210813

CH_3–$S(O)_2O^+$ (3-C_3V)

MeSO3+ with enforced symmetry
E(RM062X) = -663.014291053

Zero-point correction= 0.047665 (Hartree/Particle)
Thermal correction to Energy= 0.052433

Thermal correction to Enthalpy= 0.053377
Thermal correction to Gibbs Free Energy= 0.019393
Sum of electronic and zero-point Energies= -662.966627
Sum of electronic and thermal Energies= -662.961858
Sum of electronic and thermal Enthalpies= -662.960914
Sum of electronic and thermal Free Energies= -662.994899

E (Thermal) CV S
KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin
Total 32.902 15.213 71.527

S,1,sc5,2,sch2
H,1,hc2,2,hch3,3,dih1,0
H,1,hc2,2,hch3,3,-dih1,0
O,3,os6,1,osc6,2,dih6,0
O,3,os6,1,osc6,4,dih6,0
O,3,os6,1,osc6,5,dih6,0

hc2=1.093856
sch2=107.136
hch3=111.714
dih1=117.017
os6=1.484186
osc6=112.877
sc5=1.759173

$CH_3–S(O)_2O^+$ (3-*C_S*)

E(RM062X) = -663.090258889

Zero-point correction= 0.049998 (Hartree/Particle)
Thermal correction to Energy= 0.055444
Thermal correction to Enthalpy= 0.056388
Thermal correction to Gibbs Free Energy= 0.021197
Sum of electronic and ZPE= -663.040261
Sum of electronic and thermal Energies= -663.034815
Sum of electronic and thermal Enthalpies= -663.033871
Sum of electronic and thermal Free Energies= -663.069062

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 34.791 17.960 74.065

S,0,-3.6848975658,1.398170393,-0.319246526
O,0,-2.4552741865,0.4613648936,0.0162204171
O,0,-3.5572957,2.7924171131,-0.5247398956
O,0,-3.5257134099,0.7189654942,1.1001385158
C,0,-4.8864953755,0.5293419652,-1.2970002333
H,0,-4.82895468,-0.5202156223,-1.0003860629
H,0,-5.8540255847,0.9881602903,-1.0677966601
H,0,-4.6072909475,0.6972321129,-2.3423520448

$CH_3–S(O)_2O^+$ (3-*open shell*)

E(UM062X) = -663.057807276

Zero-point correction= 0.047178 (Hartree/Particle)
Thermal correction to Energy= 0.053279
Thermal correction to Enthalpy= 0.054224
Thermal correction to Gibbs Free Energy= 0.017638
Sum of electronic and ZPE= -663.010629
Sum of electronic and thermal Energies= -663.004528
Sum of electronic and thermal Enthalpies= -663.003584
Sum of electronic and thermal Free Energies= -663.040170

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 33.433 19.667 77.001

C,0,0.0119267749,0.0018026077,-0.0438574186
H,0,-0.014714809,-0.0096631511,1.0539634392
S,0,1.7296979127,0.0888827623,-0.4448692198
H,0,-0.4010565474,-0.9219945841,-0.4626201315
H,0,-0.4654180039,0.8988443185,-0.4507786619
O,0,1.6343546098,-0.0315882801,-2.0252599263
O,0,2.5061100808,1.1840649756,0.0562234702
O,0,2.4517999821,-1.2104486488,0.0536984487

$MeOSO_3H_2^+$ (4)

E(RM062X) = -739.657035490

Zero-point correction= 0.078803 (Hartree/Particle)
Thermal correction to Energy= 0.086169
Thermal correction to Enthalpy= 0.087113
Thermal correction to Gibbs Free Energy= 0.047220
Sum of electronic and ZPE= -739.578233
Sum of electronic and thermal Energies= -739.570866
Sum of electronic and thermal Enthalpies= -739.569922
Sum of electronic and thermal Free Energies= -739.609815

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 54.072 24.857 83.962

C,0,0.0124793249,0.0373247188,-0.026662525
H,0,-0.1821201077,0.3589238518,0.9922491544
H,0,1.0649282068,0.134733805,-0.289177555
H,0,-0.3876936642,-0.9570253477,-0.2189456664
O,0,-0.771260983,1.0124676622,-0.8355889887
S,0,-0.6401214823,0.9901069857,-2.3579044337
O,0,-1.5500891844,2.1653052719,-2.7940395243
O,0,0.6777398465,0.9993702621,-2.8935849788
O,0,-1.5057646363,-0.2367322108,-2.7481797378
H,0,-1.0950992239,3.0328965513,-2.8208612243
H,0,-1.3793190963,-0.5391795503,-3.6716325205

$MeOSO_2^+$ (5)

E(RM062X) = -663.180387009

Zero-point correction= 0.051896 (Hartree/Particle)
Thermal correction to Energy= 0.057739
Thermal correction to Enthalpy= 0.058683
Thermal correction to Gibbs Free Energy= 0.021281
Sum of electronic and ZPE= -663.128492
Sum of electronic and thermal Energies= -663.122648
Sum of electronic and thermal Enthalpies= -663.121704
Sum of electronic and thermal Free Energies= -663.159106

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 36.232 17.641 78.719

S,0,-3.1568910187,1.3775328088,-0.0060031696
O,0,-2.0539266921,0.6410991158,-0.5101943323
O,0,-3.952553409,2.3728132413,-0.6172334251
O,0,-3.5729047425,1.0675081925,1.4189692713
C,0,-2.8519798784,0.0321685244,2.2525195598
H,0,-1.8189880392,0.3562758855,2.3612107629
H,0,-3.4093995032,0.0811797876,3.1843157815
H,0,-2.9548017171,-0.9271745559,1.7494765514

MSA

E(RM062X) = -664.180265336

Zero-point correction= 0.062429 (Hartree/Particle)
Thermal correction to Energy= 0.068293
Thermal correction to Enthalpy= 0.069237
Thermal correction to Gibbs Free Energy= 0.033305
Sum of electronic and ZPE= -664.117836
Sum of electronic and thermal Energies= -664.111972
Sum of electronic and thermal Enthalpies= -664.111028
Sum of electronic and thermal Free Energies= -664.146960

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	42.854	19.832	75.625

O,0,-0.627559728,1.2247152057,-0.5815035011
S,0,-0.5897261596,1.1356692236,-2.0221285008
O,0,-1.4774270754,2.352003686,-2.6306735891
O,0,0.6713688392,1.1412830768,-2.7427277418
C,0,-1.584934708,-0.2406906765,-2.5393858279
H,0,-0.8953923338,2.9002897515,-3.1815191844
H,0,-2.581127144,-0.1137130135,-2.1164550266
H,0,-1.6100532999,-0.2605523061,-3.6279382316
H,0,-1.1087433907,-1.1373099475,-2.1413093967

Methane

E(RM062X) = -40.4879431267

Zero-point correction= 0.045196 (Hartree/Particle)
Thermal correction to Energy= 0.048063
Thermal correction to Enthalpy= 0.049007
Thermal correction to Gibbs Free Energy= 0.025532
Sum of electronic and ZPE= -40.442747
Sum of electronic and thermal Energies= -40.439880
Sum of electronic and thermal Enthalpies= -40.438936
Sum of electronic and thermal Free Energies= -40.462411

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	30.160	6.456	49.407

C,0,-0.0000010571,0.,0.0000045306
H,0,-0.0000093302,-0.0000000001,1.0907377561
H,0,1.0283397911,0.0000000001,-0.3635858038
H,0,-0.5141647543,-0.890576056,-0.3635762055
H,0,-0.5141647544,0.890576056,-0.3635762054

CH_3• (methyl radical)

E(UM062X) = -39.8118973333

Zero-point correction= 0.029906 (Hartree/Particle)
Thermal correction to Energy= 0.033036
Thermal correction to Enthalpy= 0.033980
Thermal correction to Gibbs Free Energy= 0.011107
Sum of electronic and ZPE= -39.781992
Sum of electronic and thermal Energies= -39.778862
Sum of electronic and thermal Enthalpies= -39.777918
Sum of electronic and thermal Free Energies= -39.800790

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	20.730	7.569	48.139

C,0,-4.6184197542,-2.5947480058,3.5830395646
H,0,-4.8672805327,-2.3922552657,4.6143087041
H,0,-5.4017508147,-2.6708254495,2.8434074214
H,0,-3.5860617921,-2.7188049936,3.2909814593

Complex of CH_3• with SO_3

E(UM062X) = -663.470651495

Zero-point correction= 0.046747 (Hartree/Particle)
Thermal correction to Energy= 0.053367
Thermal correction to Enthalpy= 0.054311
Thermal correction to Gibbs Free Energy= 0.015805
Sum of electronic and ZPE= -663.423904
Sum of electronic and thermal Energies= -663.417285
Sum of electronic and thermal Enthalpies= -663.416341
Sum of electronic and thermal Free Energies= -663.454846

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	33.488	20.912	81.042

S,0,-3.4313258564,1.3273251405,0.0119872905
O,0,-2.4184504068,0.6356288526,-0.75620063
O,0,-3.7782664877,2.6875605483,-0.3400092449
O,0,-3.7944847123,0.8216163477,1.3185275211
C,0,-5.2428897838,0.3525855521,-1.1019738268
H,0,-5.0184149273,-0.6805711293,-0.8655797159
H,0,-6.0338309585,0.8454063692,-0.5495362294
H,0,-5.0086288673,0.714329319,-2.0959301647

TS for addition of CH_3• to SO_3 (6)

E(UM062X) = -663.469397802

Zero-point correction= 0.047402 (Hartree/Particle)
Thermal correction to Energy= 0.052825
Thermal correction to Enthalpy= 0.053769
Thermal correction to Gibbs Free Energy= 0.017970
Sum of electronic and ZPE= -663.421996
Sum of electronic and thermal Energies= -663.416573
Sum of electronic and thermal Enthalpies= -663.415629
Sum of electronic and thermal Free Energies= -663.451428

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	33.148	17.907	75.346

S,0,-3.3913690305,1.3614505216,-0.0253275714
O,0,-2.2826009944,0.7138773973,-0.7035416882
O,0,-3.6456820852,2.7675889912,-0.2837609059
O,0,-3.7984460042,0.8224054926,1.2900793097
C,0,-4.9984199037,0.4784709291,-0.9239547479
H,0,-4.8455310296,-0.5796088742,-0.7384257271
H,0,-5.8499812173,0.9338959268,-0.4292218141
H,0,-4.7873102151,0.8249951856,-1.9343922751

methanesulfinicacid (CH_3OSO_2H)

E(RM062X) = -664.184005322

Zero-point correction= 0.062090 (Hartree/Particle)
Thermal correction to Energy= 0.068270
Thermal correction to Enthalpy= 0.069214
Thermal correction to Gibbs Free Energy= 0.032248
Sum of electronic and ZPE= -664.121916
Sum of electronic and thermal Energies= -664.115736
Sum of electronic and thermal Enthalpies= -664.114791
Sum of electronic and thermal Free Energies= -664.151757

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	42.840	20.057	77.800

S,0,-2.9244513774,2.312308065,0.5214546603
O,0,-1.597248005,1.8400621346,0.101396428
O,0,-3.9519789536,1.6163945089,-0.5648430852
O,0,-3.3598899428,1.4796765288,1.8496394962
C,0,-3.0829316138,0.0713884029,1.8684442298
H,0,-2.0391059233,-0.1138818597,1.6058390954
H,0,-3.277801647,-0.248864321,2.8903615095
H,0,-3.7551750085,-0.4483927304,1.1807888827
H,0,-3.4287085286,1.015973271,-1.1237022167

methanesulfonyl radical (CH_3SO_3•)

E(UM062X) = -663.490740842

Zero-point correction= 0.049187 (Hartree/Particle)
Thermal correction to Energy= 0.054206
Thermal correction to Enthalpy= 0.055150
Thermal correction to Gibbs Free Energy= 0.020199
Sum of electronic and ZPE= -663.441554
Sum of electronic and thermal Energies= -663.436535
Sum of electronic and thermal Enthalpies= -663.435590
Sum of electronic and thermal Free Energies= -663.470542

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	34.015	16.713	73.561

S,0,-3.5421666854,1.2420945795,-0.2563509028
O,0,-2.320857872,0.482462575,-0.4460448163
O,0,-3.5763249171,2.6838912876,-0.4134344738
O,0,-3.9748107292,0.9733326505,1.2305972348
C,0,-4.8313261848,0.5215009132,-1.2425926294
H,0,-4.8762725845,-0.5450513803,-1.0202013564
H,0,-5.7691778399,1.0206346923,-0.9970084368
H,0,-4.5690606788,0.6865712733,-2.2890376394

TS for H-Atom abstraction from methane by CH_3SO_3•

E(UM062X) = -703.969186706

Zero-point correction= 0.093423 (Hartree/Particle)
Thermal correction to Energy= 0.102131
Thermal correction to Enthalpy= 0.103075
Thermal correction to Gibbs Free Energy= 0.058712
Sum of electronic and ZPE= -703.875763
Sum of electronic and thermal Energies= -703.867056
Sum of electronic and thermal Enthalpies= -703.866112
Sum of electronic and thermal Free Energies= -703.910475

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	64.088	28.067	93.370

S,0,-3.610015107,0.6182911302,-0.3453001373
O,0,-3.2746927236,-0.7239061615,0.0894661709
O,0,-2.5978667997,1.4451503121,-0.9723465879
O,0,-4.3015332677,1.4251638192,0.8871000116
C,0,-5.0806769754,0.5908691746,-1.3568262696
H,0,-5.8563881813,0.034081128,-0.8334882443
H,0,-5.3799222092,1.6162152849,-1.5704625765
H,0,-4.782751177,0.0773057778,-2.2735293227
H,0,-3.2024342058,1.399932876,1.9796279796
C,0,-2.1869539524,1.1732578264,2.4587490699
H,0,-1.422371354,1.3341193839,1.7002100823
H,0,-2.1016772319,1.877766495,3.2864310566
H,0,-2.2242394849,0.1356863633,2.7855549475

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