New particle formation from the reactions of ozone with indene and styrene.

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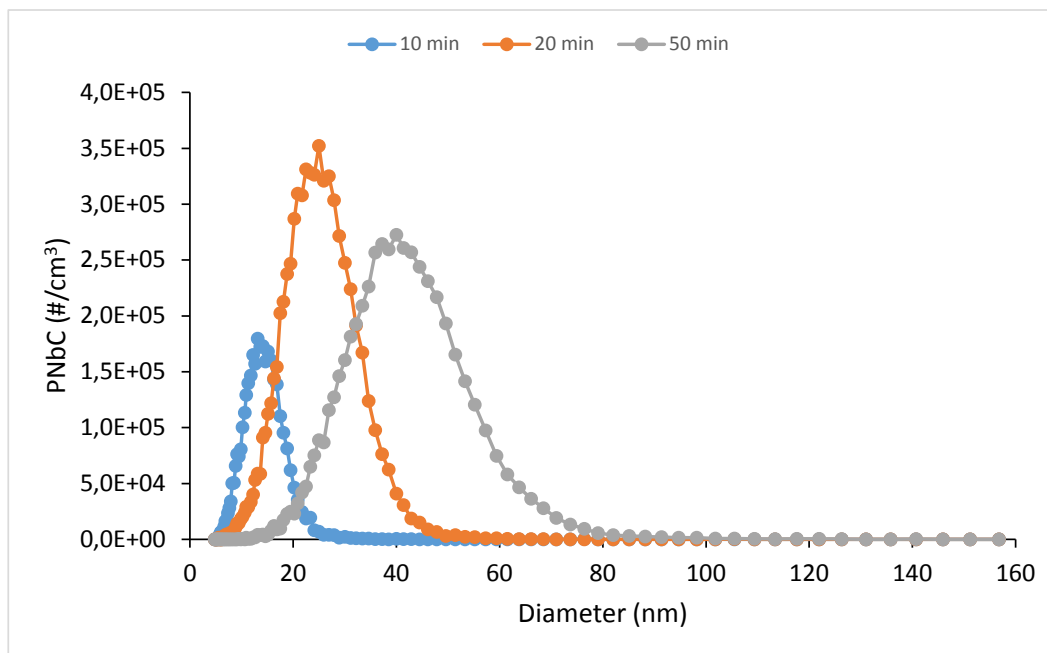
SUPPLEMENTARY MATERIAL

Fig. S1. Particle size distributions at different times of reaction. Initial concentrations of reagents: indene and SO_2: 30ppb. Ozone 60ppb. RH=0.
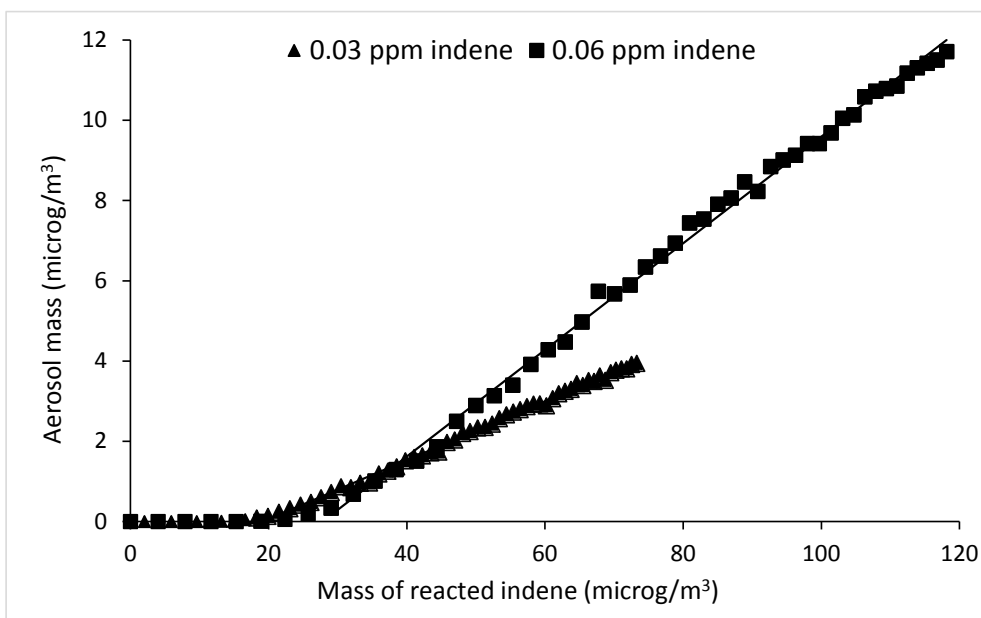

Fig. S2. Mass of formed aerosol versus the mass concentration of reacted indene. Initial concentrations of reagents: SO_2 30ppb, Ozone 60ppb, RH=0.
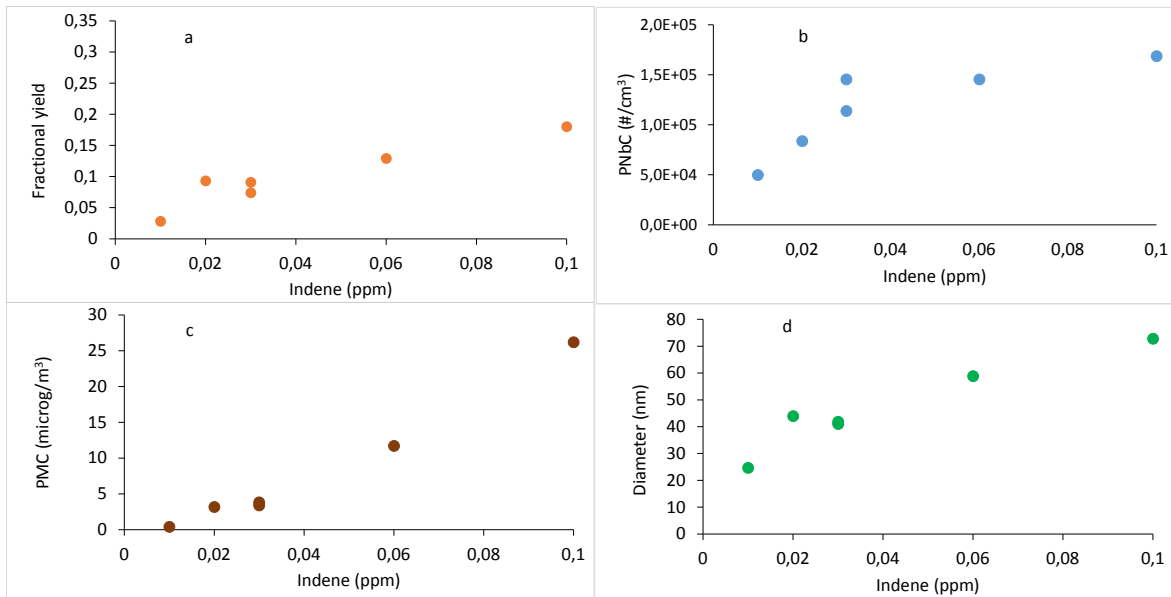
Fig. S3. Effect of [indene] on the production of SOA for a series of experiments with initial concentrations of ozone=60ppb and SO_2=30ppb. RH=0. a) Fractional yield. b) Maximum particle number concentration recorded during the experiment. c) PMC at reaction time =50'. d) Average particle diameter at reaction time =50'.
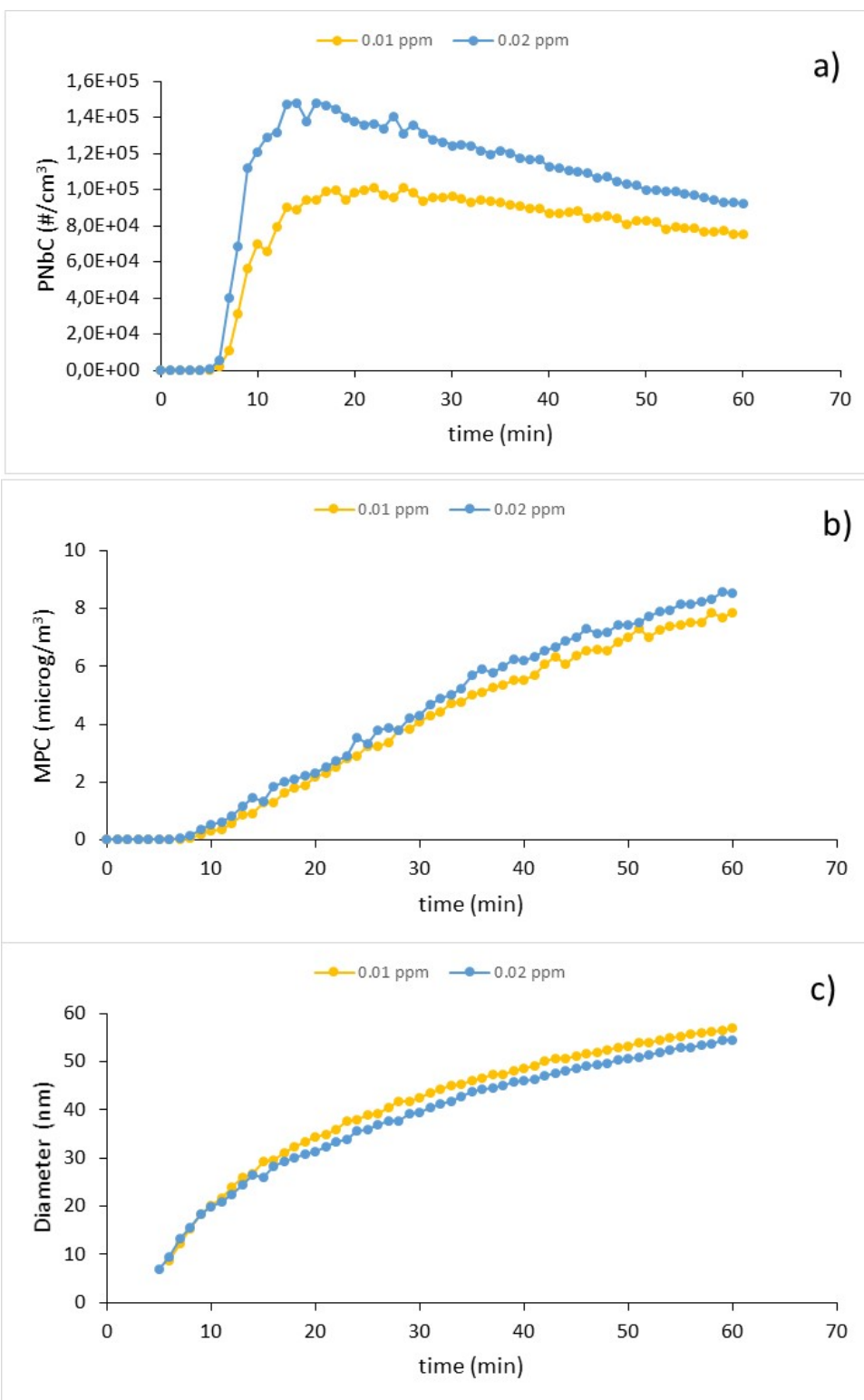
Fig. S4. Effect of [SO$_2$] on the production of SOA. Time profiles for a) PNbC, b) PMC and c) average particle diameter. For this series of experiments [indene]=30 ppb, [ozone]= 60ppb, RH=0.
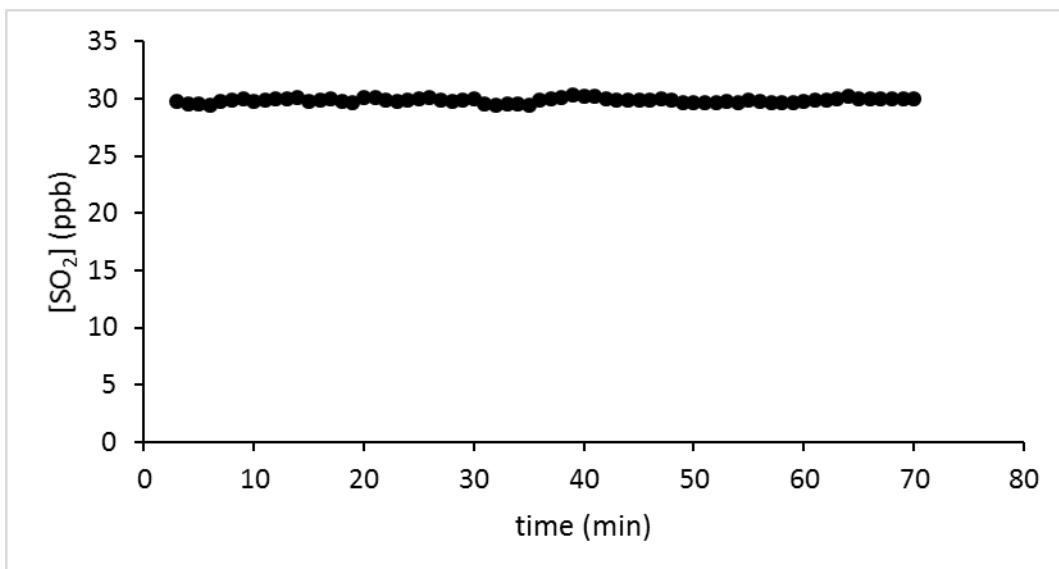
Fig. S5. SO_2 profile during ozonolysis reactions of indene. Initial concentrations: [indene]=500 ppb, [Ozone]= 500ppb, RH=0.

a

Styrene

PO

TSba

TSb

sCl-H$_2$COO

sCl-PhCHOO
(phenyl formate)
syn

sCl-PhCHOO
(phenyl formate)
anti

Adduct
H$_2$COO-SO$_2$

Adduct
PhCHOO-SO$_2$

TS1
H$_2$CO—OSO$_2$

TS2
HCOOH--SO$_2$

TS3
PhOCHO—SO$_2$

TS2
PhCHOO—SO$_2$

TS1
PhCHO—OSO$_2$

Formaldehyde

Formic acid

PhCHO
(Benzaldehyde)

PhCOOH
(Benzoic acid)

PhOCHO
(Formiato de bencilo)

b

Indene PO TSa TSb sCI-Indene1 syn sCI-Indene1 anti sCI-Indene2 syn sCI-Indene2 anti

SOZ Sci-Indene1-SO$_2$ SOZ Sci-Indene2-SO$_2$ TS1 Sci_Indene1-SO$_2$ TS2 Sci_Indene1-SO$_2$ TS3 Sci-Indene1-SO$_2$ TS1 Sci_Indene2-SO2 TS2 Sci_Indene2-SO2 TS3 sCI_Indene2-SO$_2$

Aldehyde-Indene1 (2-(2-oxoethyl)-benzaldehyde) Acid-Indene1 ((2-formylphenyl)-acetic acid) Ester-Indene1 (2-(oxomethyl)-benzylformate) Aldhyde-Indene2 (2-(2-oxoethyl)-benzaldehyde) Acid-Indene2 (2-(2-oxo-ethyl)-benzoic acid) Ester-Indene2 (2-(2-oxo-ethyl)-Phenilformate)
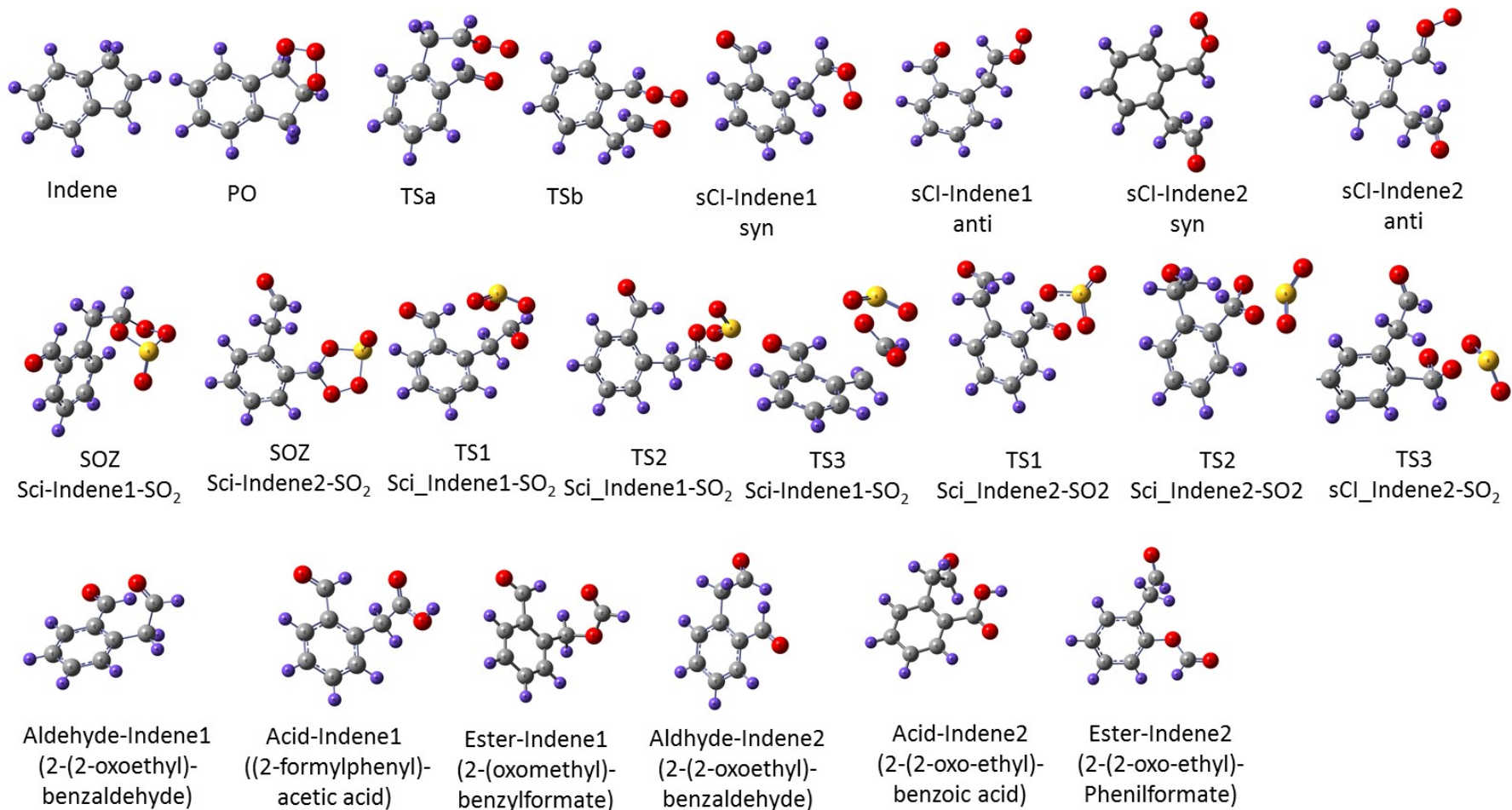
Fig. S6. Optimized structures, including reactants, products, secondary ozonide SOZ and transitions states ST, calculated at the BMK/6-311++G(2df,2pd) level of theory. a) Styrene/O$_3$/SO$_2$ system and b) Indene/O$_3$/SO$_2$ system.
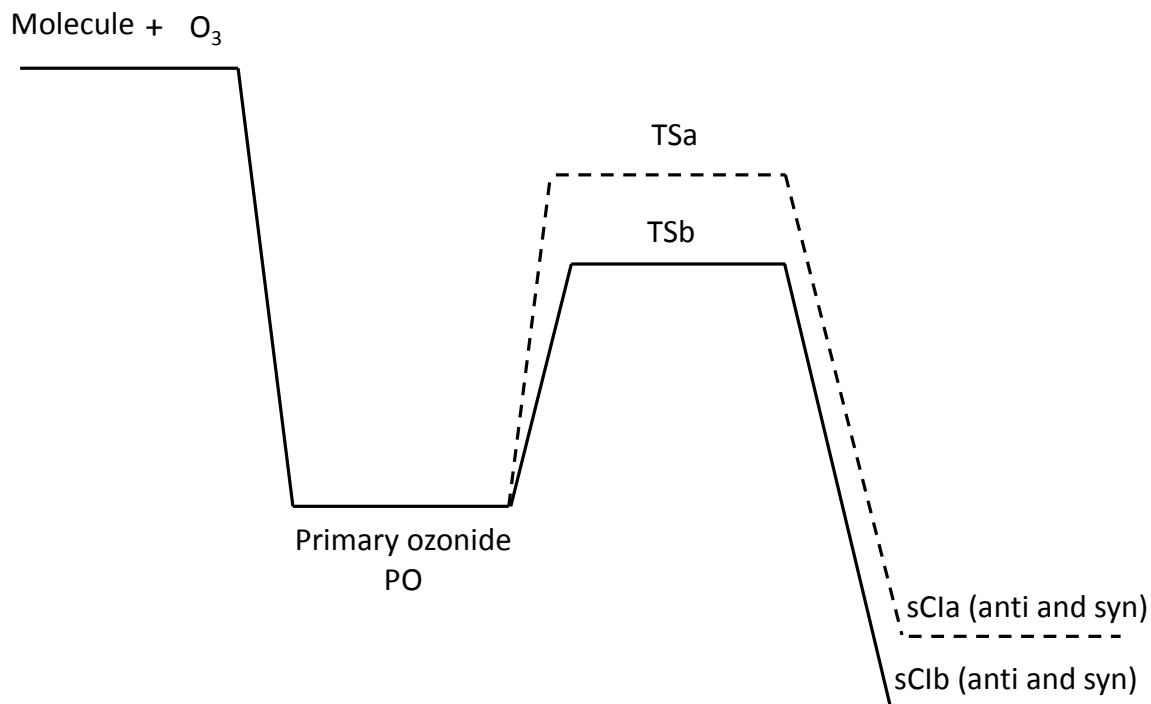
Fig. S7. General schematic potential energy surfaces representing the sCI formation in the ozone/Styrene and ozone/Indene systems. TSa is the transition state to form sCI-H_2COO in styrene system or sCI-Indene1 in the case of indene (sCIa). TSb is the transition state to form sCI-PhCHOO for styrene system or sCI-Indene2 in the case of Indene system (sCIb).

Table S1. Relative enthalpies at 0 K (in kcal mol^{-1}) among molecule + O_3, adducts (primary cyclic ozonide PO), transition states (TS) and products, calculated at the BMK/6-311++G(2df,2pd) level of theory.

System	Adduct (PO)	TSa	TSb	sCIa	sCIa syn	sCIa anti	sCIb syn	sCIb anti
Styrene + O_3	0.0	-63.3	-43.5	-44.2	-70.0	-	-	-71.9	-71.4
Indene + O_3	0.0	-62.8	-42.3	-43.3	-	-74.3	-75.3	-74.1	-74.6

g

h

i
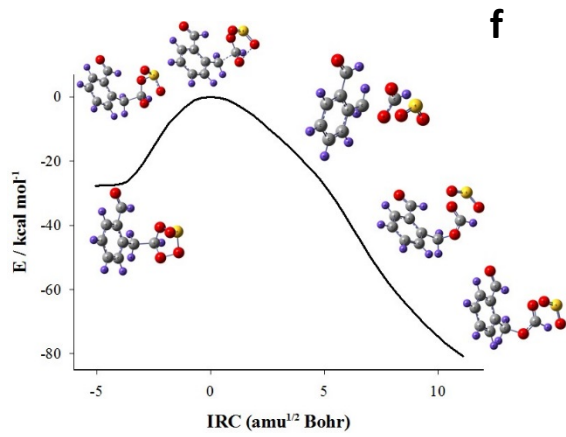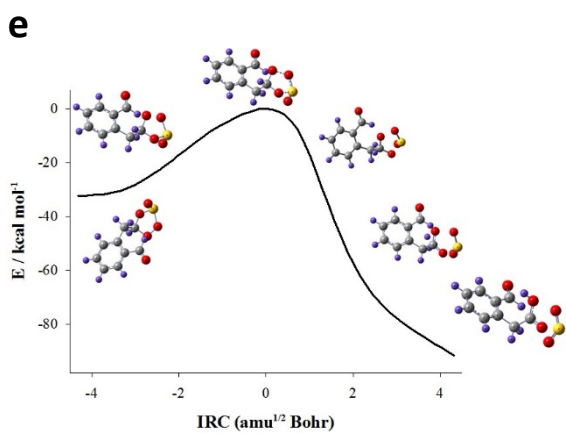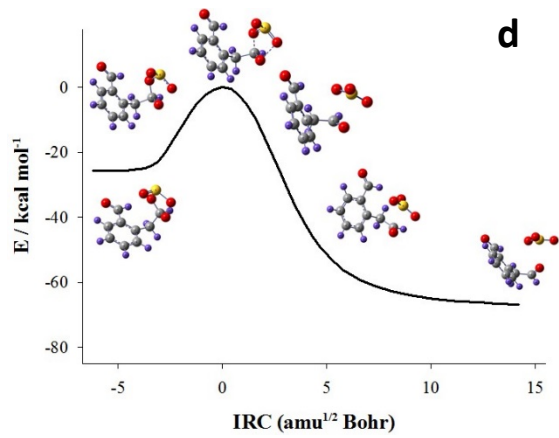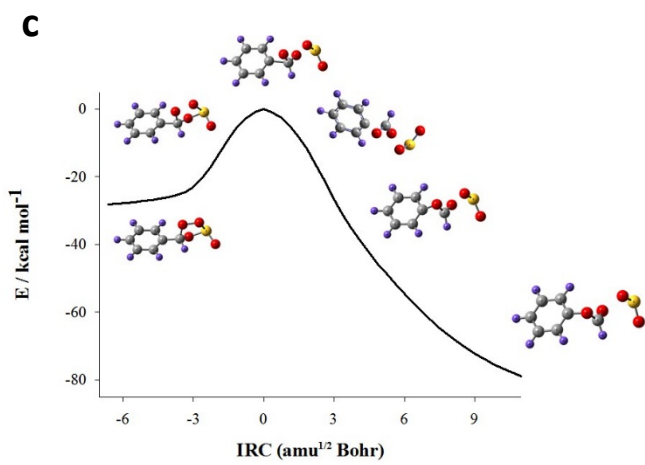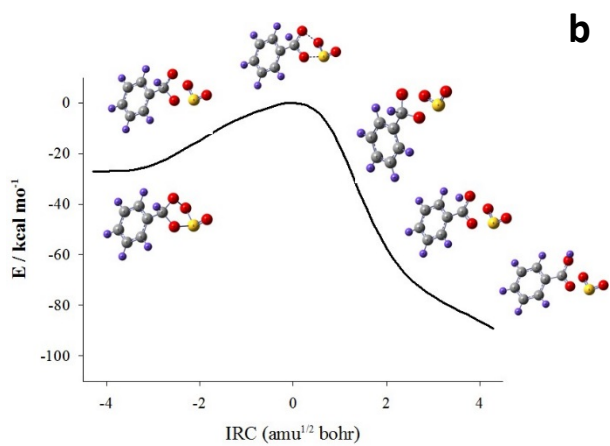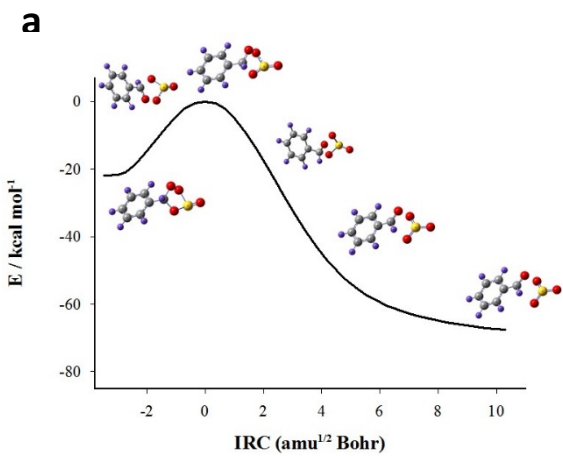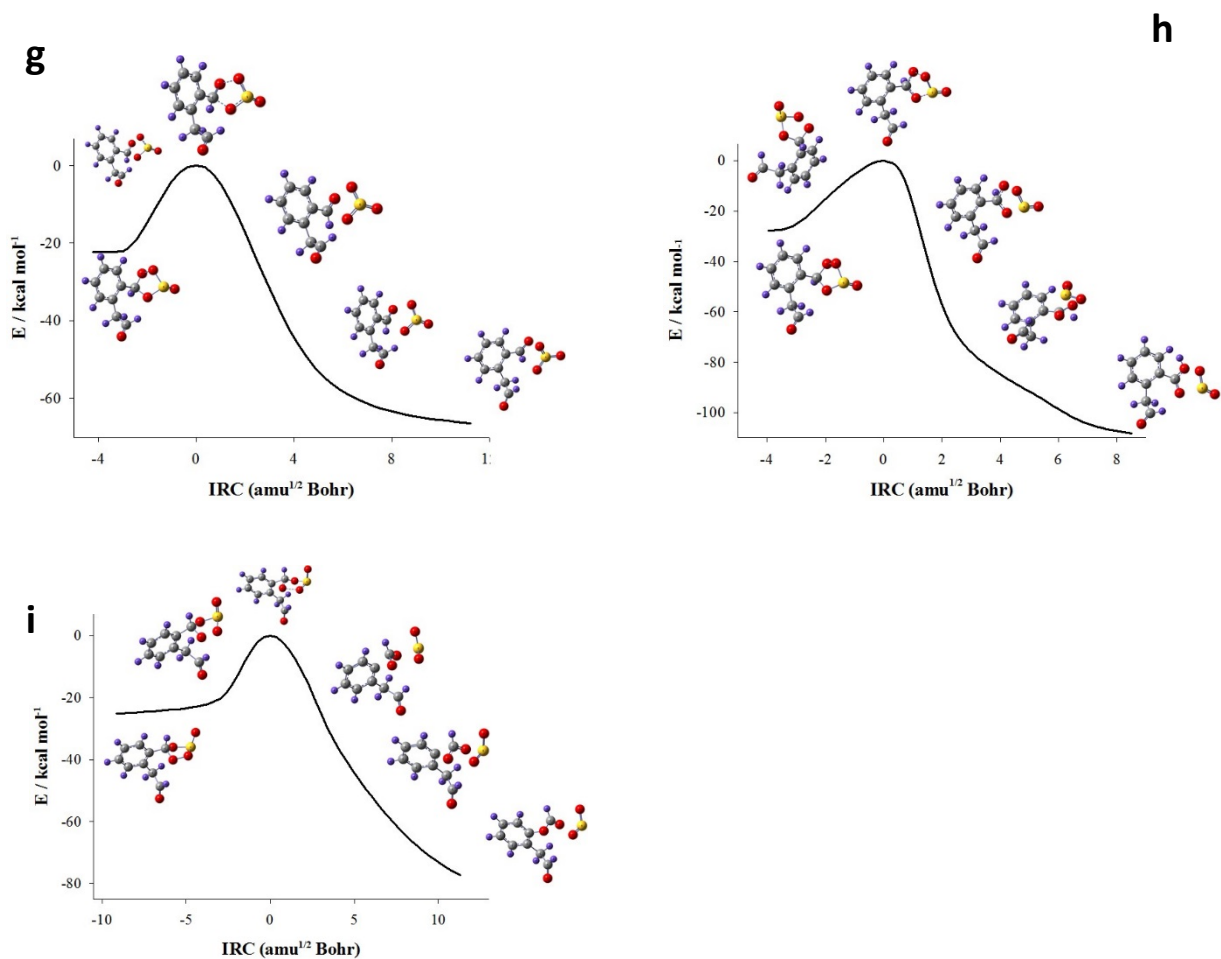
Fig. S8. Relative energy along the intrinsic reaction coordinate (IRC) for the studied sCI + SO$_2$ reactions. a) (R1) in sCI-PhCHOO + SO$_2$, b) (R2) in sCI-PhCHOO +SO$_2$, c) (R3) in sCI-PhCHOO +SO$_2$, d) (R1) in sCI-Indene1 +SO$_2$, e) (R2) in sCI-Indene1 +SO$_2$, f) (R3) in sCI-Indene1 + SO$_2$, g) (R1) in sCI-Indene2 + SO$_2$, h) (R2) in sCI-Inden2 +SO$_2$ and i) (R3) in sCI-Indene2 + SO$_2$.
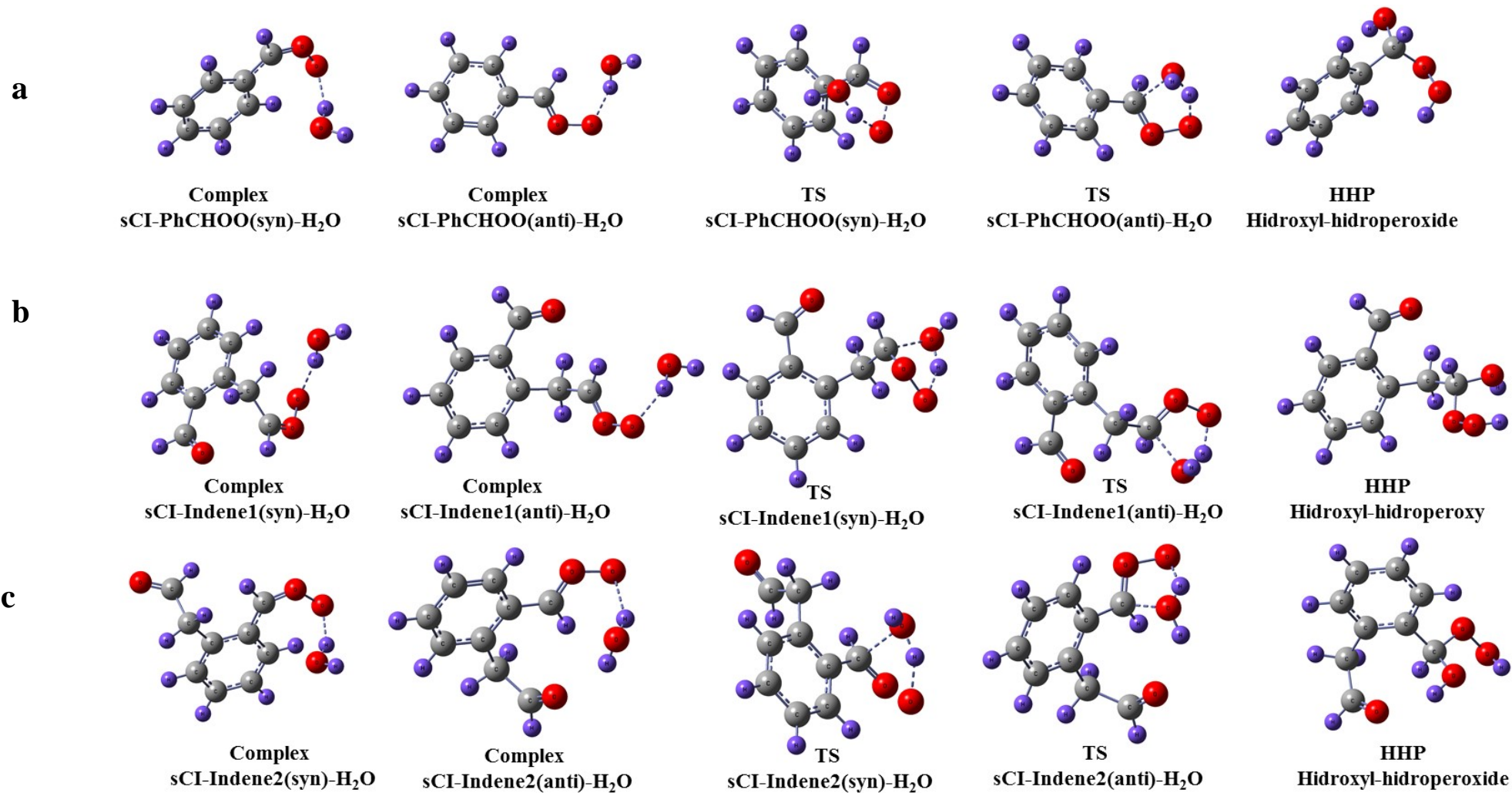
Fig. S9. Optimized structures, including complex, products, and transitions states TS, calculated at the BMK/6-311++G(2df,2pd) level of theory. a) sCI-PhCHOO/H_2O system, b) sCI-Indene1/H_2O system and c) sCI-Indene2/H_2O system.
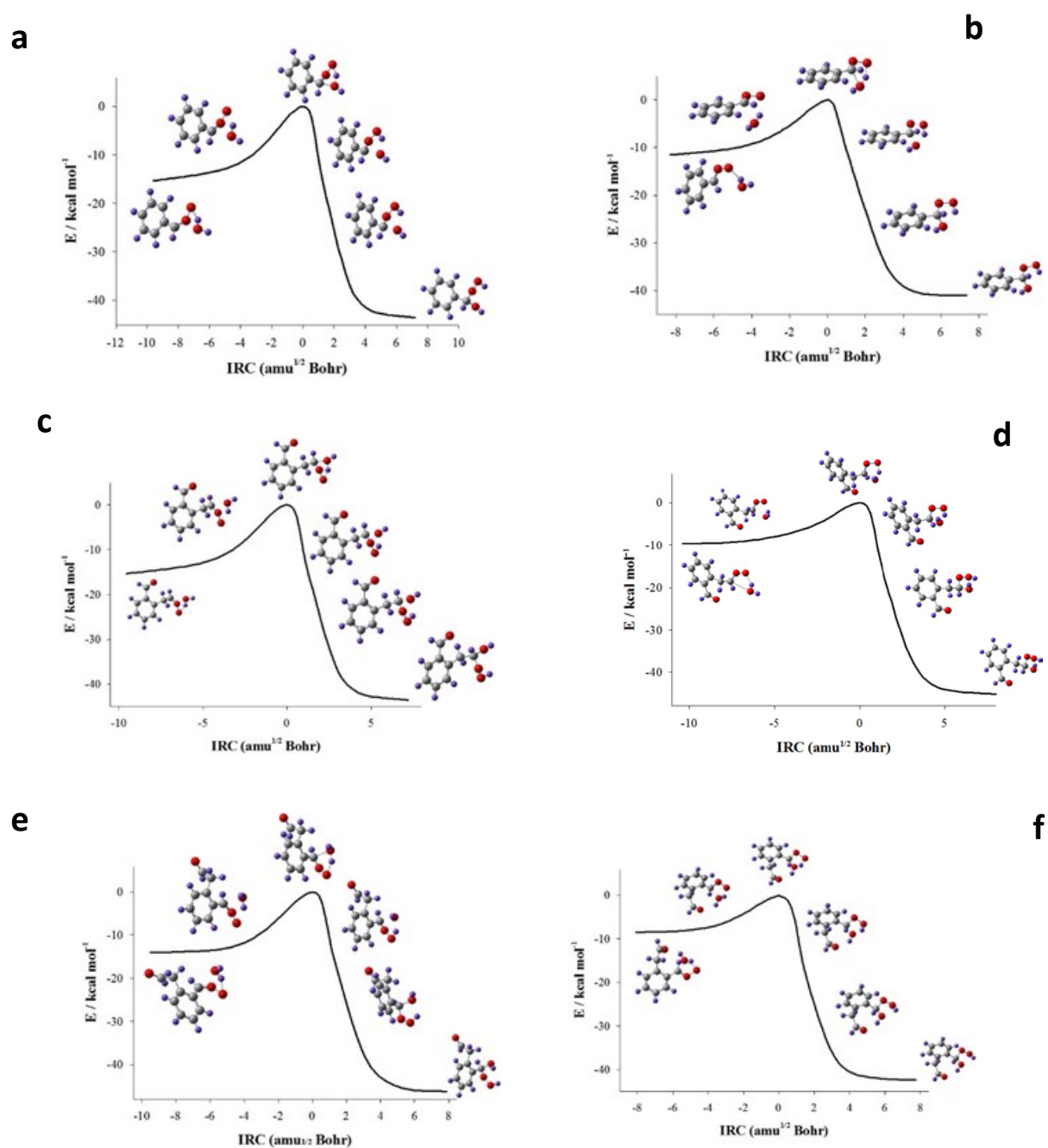
Fig. S10. Relative energy along the intrinsic reaction coordinate (IRC) for sCI + H_2O reactions. a) sCI-PhCHOOsyn + H_2O b) sCI-PhCHOOanti + H_2O c) sCI-Indene1syn + H_2O d) sCI-Indene1anti + H_2O e) sCI-Indene2syn + H_2O f) sCI-Indene2anti + H_2O

APENDIX A

Vibrational frequencies, rotational constants, and energies of the molecular species involved in the Styrene-Indene/O_3/SO_2-H_2O reactions at BMK/6-311++G(2df,2pd) level of theory

H_2COO

Frequencies (cm^{-1}): 545, 694, 956, 1021, 1280, 1453, 1647, 3128, 3281

Rotational constants (GHZ):   82.27800   12.60305   10.92899

Zero-point correction=   0.031907 (Hartree/Particle)

 Thermal correction to Energy=   0.035146

 Thermal correction to Enthalpy=   0.036090

 Thermal correction to Gibbs Free Energy=   0.007869

 Sum of electronic and zero-point Energies=   -189.515909

 Sum of electronic and thermal Energies=   -189.512670

 Sum of electronic and thermal Enthalpies=   -189.511726

 Sum of electronic and thermal Free Energies=   -189.539947

SO_2H_2COO (SOZ)

Frequencies: 140, 296, 396, 483, 568, 679, 722, 749, 924, 1008, 1092, 1157, 1253, 1324, 1412, 1537, 3065, 3157

Rotational constants (GHZ):   6.22472   3.17541   2.64168

Zero-point correction=   0.045482 (Hartree/Particle)

 Thermal correction to Energy=   0.050615

 Thermal correction to Enthalpy=   0.051559

 Thermal correction to Gibbs Free Energy=   0.016428

 Sum of electronic and zero-point Energies=   -738.085010

 Sum of electronic and thermal Energies=   -738.079877

 Sum of electronic and thermal Enthalpies=   -738.078933

 Sum of electronic and thermal Free Energies=   -738.114064

ST1_H_2COO_SO_3

Frequencies: -654, 148, 189, 307, 454, 522, 544, 674, 870, 1004, 1052, 1165, 1296, 1342, 1357, 1492, 2997, 3098

Rotational constants (GHZ):   6.18631   2.88063   2.50738

Zero-point correction=   0.042177 (Hartree/Particle)

 Thermal correction to Energy=   0.047612

Thermal correction to Enthalpy=   0.048556

Thermal correction to Gibbs Free Energy=   0.012717

Sum of electronic and zero-point Energies=   -738.048698

Sum of electronic and thermal Energies=   -738.043263

Sum of electronic and thermal Enthalpies=   -738.042319

Sum of electronic and thermal Free Energies=   -738.078158

ST2_H$_2$COO_SO$_2$

Frequencies: -972, 146, 257, 293, 412, 449, 494, 545, 735, 876, 1057, 1203, 1257, 1340, 1348, 1435, 2506, 3027

Rotational constants (GHZ):   6.04210   2.77440   2.38272

Zero-point correction=   0.039594 (Hartree/Particle)

 Thermal correction to Energy=   0.045209

 Thermal correction to Enthalpy=   0.046153

 Thermal correction to Gibbs Free Energy=   0.010078

 Sum of electronic and zero-point Energies=   -738.040128

 Sum of electronic and thermal Energies=   -738.034513

 Sum of electronic and thermal Enthalpies=   -738.033569

 Sum of electronic and thermal Free Energies=   -738.069644

H$_2$CO

Frequencies: 1225, 1289, 1557, 1883, 2924, 2995

Rotational constants (GHZ):   283.93174   39.55694   34.71983

Zero-point correction=   0.027069 (Hartree/Particle)

 Thermal correction to Energy=   0.029933

 Thermal correction to Enthalpy=   0.030878

 Thermal correction to Gibbs Free Energy=   0.005426

 Sum of electronic and zero-point Energies=   -114.455977

 Sum of electronic and thermal Energies=   -114.453113

 Sum of electronic and thermal Enthalpies=   -114.452169

 Sum of electronic and thermal Free Energies=   -114.477621

HCOOH

Frequencies: 528, 683, 1082, 1149, 1292, 1443, 1926, 3008, 3903

Rotational constants (GHZ):   88.39375   11.86757   10.46285

Zero-point correction= 0.034208 (Hartree/Particle)

Thermal correction to Energy= 0.037430

Thermal correction to Enthalpy= 0.038374

Thermal correction to Gibbs Free Energy= 0.010154

Sum of electronic and zero-point Energies= -189.700564

Sum of electronic and thermal Energies= -189.697341

Sum of electronic and thermal Enthalpies= -189.696397

Sum of electronic and thermal Free Energies= -189.724618

Styrene

Frequencies: 84, 230, 261, 418, 453, 461, 566, 632, 677, 731, 790, 823, 874, 964, 982, 1014, 1016, 1038, 1044, 1063, 1063, 1119, 1182, 1222, 1230, 1303, 1342, 1381, 1471, 1493, 1543, 1623, 1649, 1695, 3150, 3159, 3177, 3184, 3193

Rotational constants (GHZ): 5.19667 1.54234 1.18935

Zero-point correction= 0.134311 (Hartree/Particle)

Thermal correction to Energy= 0.140856

Thermal correction to Enthalpy= 0.141800

Thermal correction to Gibbs Free Energy= 0.103514

Sum of electronic and zero-point Energies= -309.380097

Sum of electronic and thermal Energies= -309.373552

Sum of electronic and thermal Enthalpies= -309.372608

Sum of electronic and thermal Free Energies= -309.410894

Cyclic ozonide (PO)

Frequencies: 57, 64, 130, 227, 314, 341, 419, 422, 544, 607, 635, 731, 736, 772, 799, 807, 866, 886, 963,   983, 1005, 1019, 1021, 1042, 1047, 1052, 1066, 1079, 1112, 1183, 1201, 1232, 1263. 1305, 1313, 1350, 1377, 1405, 1499, 1531, 1537, 1635, 1653, 3065, 3078, 3160, 3173, 3181, 3191, 3200, 3207
Rotational constants (GHZ): 3.05384 0.66956 0.62621
Zero-point correction= 0.149193 (Hartree/Particle)

Thermal correction to Energy= 0.157741

Thermal correction to Enthalpy= 0.158686

Thermal correction to Gibbs Free Energy= 0.114476

Sum of electronic and zero-point Energies= -534.852162

Sum of electronic and thermal Energies= -534.843614

Sum of electronic and thermal Enthalpies= -534.842670

Sum of electronic and thermal Free Energies= -534.886879

ST_Ozonide_cyclic_PhCHOO

Frequencies: -467, 49, 96, 138, 211, 253, 341, 412, 421, 449, 545, 550, 605, 636, 678,712, 786, 870, 880, 925, 952 1012, 1019, 1029, 1048, 1062, 1102, 1179, 1186, 1207, 1215, 1246, 1264, 1302, 1314, 1360, 1431, 1435, 1498, 1541, 1576, 1630, 1652, 2955, 3033, 3156, 3173, 3184, 3197, 3205, 3211

Rotational constants (GHZ):   2.88753   0.62590   0.59256

Zero-point correction=   0.145651 (Hartree/Particle)

Thermal correction to Energy=   0.154524

Thermal correction to Enthalpy=   0.155468

Thermal correction to Gibbs Free Energy=   0.110795

Sum of electronic and zero-point Energies=   -534.821704

Sum of electronic and thermal Energies=   -534.812831

Sum of electronic and thermal Enthalpies=   -534.811886

Sum of electronic and thermal Free Energies=   -534.856559

sCI-PhCHOO (syn)

Frequencies: 90, 171, 247, 322, 415, 418, 482, 575, 629, 712, 733, 793, 869, 889, 947, 960, 994, 1015, 1027, 1050, 1056, 1123, 1188, 1215, 1228, 1326, 1377, 1436, 1487, 1527, 1611, 1634, 1645, 3180, 3186, 3188, 3202, 3213, 3270
Rotational constants (GHZ):   4.17818   1.12845   0.88849
Zero-point correction=   0.114897 (Hartree/Particle)// QCISDT= -419.46696084 H0= -419.3520638

Thermal correction to Energy=   0.121893

Thermal correction to Enthalpy=   0.122837

Thermal correction to Gibbs Free Energy=   0.083117

Sum of electronic and zero-point Energies=   -420.412006

Sum of electronic and thermal Energies=   -420.405010

Sum of electronic and thermal Enthalpies=   -420.404066

Sum of electronic and thermal Free Energies=   -420.443786

sCI-PhCHOO (anti)

Frequencies: 99, 148, 188, 296, 379, 415, 441, 508, 629, 655, 713, 792, 880, 881, 970, 999, 1016, 1017, 1023, 1045, 1050, 1110, 1186, 1208, 1245, 1319, 1366, 1408, 1487, 1537, 1613, 1641, 1653, 3174, 3187, 3194, 3204, 3213, 3220

Rotational constants (GHZ):   5.20306   0.92101   0.78250

Zero-point correction=   0.114160 (Hartree/Particle)

Thermal correction to Energy=   0.121434

Thermal correction to Enthalpy=   0.122378

Thermal correction to Gibbs Free Energy=   0.082048

Sum of electronic and zero-point Energies=   -420.411174

Sum of electronic and thermal Energies=   -420.403900

Sum of electronic and thermal Enthalpies=   -420.402956

Sum of electronic and thermal Free Energies=   -420.443286

SO₂

Frequencies: 547, 1235, 1432

Rotational constants (GHZ):   59.47045   10.48214   8.91143

Zero-point correction=   0.007324 (Hartree/Particle)

 Thermal correction to Energy=   0.010369

 Thermal correction to Enthalpy=   0.011313

 Thermal correction to Gibbs Free Energy=   -0.016813

 Sum of electronic and zero-point Energies=   -548.510535

 Sum of electronic and thermal Energies=   -548.507490

 Sum of electronic and thermal Enthalpies=   -548.506545

 Sum of electronic and thermal Free Energies=   -548.534671

SO₂_sCI-Styrene (SOZ)

Frequencies: 42, 52, 128, 157, 238, 296, 408, 416, 427, 459, 544, 586, 634, 640, 687, 727, 751, 780, 786, 888, 891, 928, 970, 996, 1020, 1022, 1046, 1050, 1081, 1115, 1185, 1210, 1240,   1297, 1308, 1327, 1359, 1391, 1493, 1536, 1635, 1653, 3103, 3186, 3193, 3203, 3210, 3223

 Rotational constants (GHZ):   2.39049   0.50127   0.45994

Zero-point correction=   0.126485 (Hartree/Particle)

 Thermal correction to Energy=   0.136033

 Thermal correction to Enthalpy=   0.136977

 Thermal correction to Gibbs Free Energy=   0.089958

 Sum of electronic and zero-point Energies=   -968.965160

 Sum of electronic and thermal Energies=   -968.955612

 Sum of electronic and thermal Enthalpies=   -968.954668

 Sum of electronic and thermal Free Energies=   -969.001686

ST1_sCI-PhCHOO_aldehyde_SO₃

Frequencies: -619, 56, 67, 107, 157, 233, 268, 352, 416, 419, 474, 517, 557, 586, 633, 642, 718, 733, 805,   849, 890, 921, 976, 1020, 1027, 1034, 1047, 1053, 1110, 1141, 1184, 1210, 1219, 1256, 1315, 1324, 1369, 1427, 1498, 1544, 1635, 1654, 3027, 3183, 3188, 3203, 3213, 3221

 Rotational constants (GHZ):   2.32297   0.48580   0.45631

    1 imaginary frequencies ignored.

Zero-point correction=   0.124118 (Hartree/Particle)

 Thermal correction to Energy=   0.133745

 Thermal correction to Enthalpy=   0.134689

 Thermal correction to Gibbs Free Energy=   0.087759

 Sum of electronic and zero-point Energies=   -968.932225

 Sum of electronic and thermal Energies=   -968.922599

 Sum of electronic and thermal Enthalpies=   -968.921655

 Sum of electronic and thermal Free Energies=   -968.968585

ST2_Styrene_organic acid_SO$_2$

Frequencies: -896, 42, 59, 111, 196, 204, 230, 285, 412, 418, 449, 465, 511, 549, 563, 634, 668, 714, 754, 822, 851, 882, 914, 986, 1019, 1022, 1041, 1049, 1052, 1114, 1141, 1186, 1221, 1312, 1318, 1340, 1361, 1382, 1494, 1542, 1633, 1647, 2514, 3186, 3195, 3206, 3214, 3216,
Rotational constants (GHZ):   2.27436   0.48193   0.44594

Zero-point correction=   0.121037 (Hartree/Particle)

 Thermal correction to Energy=   0.131071

 Thermal correction to Enthalpy=   0.132015

 Thermal correction to Gibbs Free Energy=   0.084124

 Sum of electronic and zero-point Energies=   -968.927420

 Sum of electronic and thermal Energies=   -968.917387

 Sum of electronic and thermal Enthalpies=   -968.916442

 Sum of electronic and thermal Free Energies=   -968.964334

ST3_Styrene_ester_SO$_2$

Frequencies: -584, 76, 92 101, 157, 239, 264, 321, 381, 408, 425, 471, 513, 581, 622, 636, 696, 720, 784, 804, 871, 978, 1006, 1019, 1021, 1033, 1050, 1057, 1108, 1162, 1186, 1207, 1251, 1275, 1293, 1333, 1354, 1418, 1491, 1513, 1618, 1621, 3068, 3192, 3204, 3214, 3221, 3232

Rotational constants (GHZ):   2.77028   0.43594   0.41778

Zero-point correction=   0.123680 (Hartree/Particle)

 Thermal correction to Energy=   0.133442

 Thermal correction to Enthalpy=   0.134386

 Thermal correction to Gibbs Free Energy=   0.087617

 Sum of electronic and zero-point Energies=   -968.924418

 Sum of electronic and thermal Energies=   -968.914657

 Sum of electronic and thermal Enthalpies=   -968.913713

 Sum of electronic and thermal Free Energies=   -968.960482

SO₃

Frequencies: 520, 546, 546, 1149, 1484, 1490

Rotational constants (GHZ):　　　10.52783　10.50793　5.25894

Zero-point correction=　　　　　　0.013065 (Hartree/Particle)

 Thermal correction to Energy=　　　　0.016522

 Thermal correction to Enthalpy=　　　0.017467

 Thermal correction to Gibbs Free Energy=　　-0.013261

 Sum of electronic and zero-point Energies=　　-623.690125

 Sum of electronic and thermal Energies=　　-623.686668

 Sum of electronic and thermal Enthalpies=　　-623.685723

 Sum of electronic and thermal Free Energies=　　-623.716451

Aldeheyde_Styrene P1

Frequencies: 116, 215, 249, 422, 443, 471, 629, 664, 720, 784, 841, 890, 976, 1018, 1026, 1042, 1054, 1064, 1098, 1181, 1194, 1232, 1316, 1350, 1441, 1494, 1532, 1629, 1645, 1848, 2930, 3180, 3188, 3199, 3207, 3215
Rotational constants (GHZ):　　　5.25632　1.56584　1.20645

Zero-point correction=　　　　　　0.110504 (Hartree/Particle)

 Thermal correction to Energy=　　　　0.116769

 Thermal correction to Enthalpy=　　　0.117713

 Thermal correction to Gibbs Free Energy=　　0.079956

 Sum of electronic and zero-point Energies=　　-345.346933

 Sum of electronic and thermal Energies=　　-345.340668

 Sum of electronic and thermal Enthalpies=　　-345.339724

 Sum of electronic and thermal Free Energies=　　-345.377481

Organic acid_Styrene P2

Frequencies: 69, 164, 217, 388, 418, 440, 502, 587, 632, 651, 717, 752, 786, 85, 889, 992, 1020, 1030, 1047, 1050, 1100, 1140, 1185, 1199, 1222, 1315, 1354, 1403, 1492, 1533, 1632, 1648.1851, 1859, 3186, 3197, 3207, 3219, 3220, 3861,

 Rotational constants (GHZ):　　　3.90372　1.22840　0.93438

Zero-point correction=　　　　　　0.116582 (Hartree/Particle)

Thermal correction to Energy=　　　　0.123626

 Thermal correction to Enthalpy=　　　0.124570

 Thermal correction to Gibbs Free Energy=　　0.084609

 Sum of electronic and zero-point Energies=　　-420.596067

Sum of electronic and thermal Energies=   -420.589024

Sum of electronic and thermal Enthalpies=   -420.588080

Sum of electronic and thermal Free Energies=   -420.628041

Ester_Styrene P3

Frequencies: 71, 135, 179, 305, 407, 429, 464, 557, 629, 686, 724, 795, 876, 899, 948, 1019, 1021, 1032, 1047, 1076, 1100, 1172, 1180, 1203, 1286, 1303, 1360, 1638, 1646, 1907, 3032, 3190, 3199, 3206, 3213, 3221

Rotational constants (GHZ):   5.03989   0.98020   0.84156

Zero-point correction=   0.115332 (Hartree/Particle)

Thermal correction to Energy=   0.122552

Thermal correction to Enthalpy=   0.123496

Thermal correction to Gibbs Free Energy=   0.083009

Sum of electronic and zero-point Energies=   -420.566766

Sum of electronic and thermal Energies=   -420.559546

Sum of electronic and thermal Enthalpies=   -420.558602

Sum of electronic and thermal Free Energies=   -420.599089

Complex sCI-PhCHOO(syn)-H$_2$O

Frequencies: 26, 63, 127, 175, 217, 219, 260, 328, 413, 420, 482, 562, 580, 632, 703, 736, 775, 802, 857, 864, 936, 948, 979, 1014, 1024, 1040, 1051, 1116, 1184, 1205, 1230, 1332, 1357, 1454, 1484, 1522, 1611, 1638, 1659, 1790, 3177, 3186, 3191, 3201, 3213, 3277, 3662, 3986

Rotational constants (GHZ):   2.21388   0.86161   0.76243

Zero-point correction=   0.140576 (Hartree/Particle)

Thermal correction to Energy=   0.150513

Thermal correction to Enthalpy=   0.151457

Thermal correction to Gibbs Free Energy=   0.104224

Sum of electronic and zero-point Energies=   -496.818551

Sum of electronic and thermal Energies=   -496.808614

Sum of electronic and thermal Enthalpies=   -496.807670

Sum of electronic and thermal Free Energies=   -496.854903

Complex sCI-PhCHOO(anti)-H$_2$O

Frequencies: 25, 80, 87, 116, 151, 186, 269, 304, 384, 415, 455, 508, 542, 638, 659, 684, 711, 791, 883, 890, 973, 988, 1020, 1023, 1044, 1049, 1050, 1116, 1186, 1215, 1263, 1323, 1372, 1453, 1487, 1540, 1616, 1645, 1659, 1696, 3169, 3189,   3200, 3207, 3212, 3221, 3597, 3996

Rotational constants (GHZ):   2.89699   0.64166   0.52992

Zero-point correction=   0.139626 (Hartree/Particle)

Thermal correction to Energy=   0.150024

Thermal correction to Enthalpy=   0.150968

Thermal correction to Gibbs Free Energy=   0.102297

Sum of electronic and zero-point Energies=   -496.821733

Sum of electronic and thermal Energies=   -496.811335

Sum of electronic and thermal Enthalpies=   -496.810391

Sum of electronic and thermal Free Energies=   -496.859063

ST-PhCHOO(syn)-H₂O

Frequencies: -553, 54, 110, 221, 276, 294, 378, 412, 418, 513, 548, 624, 628, 703, 711, 744, 779, 861, 877, 911, 967, 1017, 1019, 1042, 1054, 1075, 1126, 1178, 1181, 1224, 1242, 1313, 1375, 1402, 1483, 1536, 1553, 1628, 1648, 1668, 2176, 3167, 3179, 3187, 3204, 3211, 3287, 3926

Rotational constants (GHZ):   2.78016   0.90687   0.78168

Zero-point correction=   0.139273 (Hartree/Particle)

Thermal correction to Energy=   0.147582

Thermal correction to Enthalpy=   0.148526

Thermal correction to Gibbs Free Energy=   0.105622

Sum of electronic and zero-point Energies=   -496.794146

Sum of electronic and thermal Energies=   -496.785837

Sum of electronic and thermal Enthalpies=   -496.784893

Sum of electronic and thermal Free Energies=   -496.827797

ST-PhCHOO(anti)-H₂O

Frequencies: -677, 61, 101, 154, 251, 322, 373, 417, 428, 510, 564, 598, 634, 651, 709, 720, 800, 884, 897, 969, 978, 1021, 1033, 1046, 1050, 1095, 1111, 1185, 1188, 1213, 1240, 1313, 1368, 1381, 1482, 1537, 1562, 1592, 1632, 1651, 1981, 3185, 3189, 3196, 3206, 3215, 3223, 3927

Rotational constants (GHZ):   3.24720   0.76494   0.69051

Zero-point correction=   0.138616 (Hartree/Particle)

Thermal correction to Energy=   0.147034

Thermal correction to Enthalpy=   0.147978

Thermal correction to Gibbs Free Energy=   0.104710

Sum of electronic and zero-point Energies=   -496.803723

Sum of electronic and thermal Energies=   -496.795305

Sum of electronic and thermal Enthalpies=   -496.794361

Sum of electronic and thermal Free Energies=   -496.837629

Product-PhCHOO(anti)-H₂O

Frequencies: 52, 100, 171, 213, 253, 279, 320, 374, 419, 465, 527, 593, 634, 658, 734, 795, 836, 889, 970, 1019, 1019, 1029, 1041, 1049, 1073, 1108, 1142, 1183, 1206, 1240, 1289, 1323, 1351, 1384, 1429, 1441, 1496, 1536, 1632, 1652, 3104, 3178, 3208, 3821, 3909

Rotational constants (GHZ):   2.45786   0.91293   0.83407

Zero-point correction=   0.142886 (Hartree/Particle)

Thermal correction to Energy=   0.151973

Thermal correction to Enthalpy=   0.152918

Thermal correction to Gibbs Free Energy=   0.108374

Sum of electronic and zero-point Energies=   -496.859962

Sum of electronic and thermal Energies=   -496.850874

Sum of electronic and thermal Enthalpies=   -496.849930

Sum of electronic and thermal Free Energies=   -496.894474

Indene

Frequencies: 199, 216, 375, 405, 437, 540, 571, 597, 736, 737, 756, 808, 840, 870, 908, 961, 965, 992, 1007, 1028, 1042, 1096, 1141, 1156, 1177, 1187, 1230, 1258, 1309, 1344, 1398, 1460, 1491, 1501, 1600, 1635, 1653, 3038, 3069, 3178, 3185, 3194, 3200, 3206, 3224

Rotational constants (GHZ):   3.78961   1.58168   1.12367

Zero-point correction=   0.141067 (Hartree/Particle)

Thermal correction to Energy=   0.147398

Thermal correction to Enthalpy=   0.148342

Thermal correction to Gibbs Free Energy=   0.110625

Sum of electronic and zero-point Energies=   -347.477687

Sum of electronic and thermal Energies=   -347.471355

Sum of electronic and thermal Enthalpies=   -347.470411

Sum of electronic and thermal Free Energies=   -347.508128

IndeneOOOcyclic (PO)

Frequencies: 60, 109, 178, 288, 328, 392, 411, 448, 524, 546, 609, 653, 728, 738, 769, 786, 850, 864, 874, 880, 909, 947, 977, 1010, 1023, 1030, 1043, 1086, 1092, 1120, 1172, 1201, 1220, 1234, 1250, 1287, 1314, 1322, 1362, 1369, 1390, 1493, 1498, 1522, 1629, 1652, 3068, 3072, 3090, 3111, 3174, 3182, 3191, 3203

Rotational constants (GHZ):   2.21530   0.74898   0.60585

Zero-point correction=   0.155546 (Hartree/Particle)

Thermal correction to Energy=   0.164015

Thermal correction to Enthalpy=   0.164959

Thermal correction to Gibbs Free Energy= 0.121367

Sum of electronic and zero-point Energies= -572.948931

Sum of electronic and thermal Energies= -572.940463

Sum of electronic and thermal Enthalpies= -572.939519

Sum of electronic and thermal Free Energies= -572.983111

ST_IndeneOOOcyclic_sCI-Indene1

Frequencies: -436, 74, 129, 202, 270, 304, 373, 416, 429, 477, 496, 540, 608, 626, 663, 712, 737, 772, 824, 846, 893, 926, 953, 995, 1033, 1037, 1046, 1106, 1117, 1170, 1177, 1195, 1229, 1254, 1276, 1304, 1323, 1339, 1356, 1430, 1476, 1491, 1512, 1521, 1626, 1649, 2924, 3066, 3109, 3175, 3180, 3189, 3200, 3208

Rotational constants (GHZ): 1.98753 0.76411 0.61967

Zero-point correction= 0.152604 (Hartree/Particle)/

Thermal correction to Energy= 0.161270

Thermal correction to Enthalpy= 0.162214

Thermal correction to Gibbs Free Energy= 0.118548

Sum of electronic and zero-point Energies= -572.916365

Sum of electronic and thermal Energies= -572.907699

Sum of electronic and thermal Enthalpies= -572.906755

Sum of electronic and thermal Free Energies= -572.950422

sCI_Indene1 (syn)

Frequencies: 46, 89, 96, 146, 191, 243, 268, 297, 433, 467, 476, 506, 518, 612, 648, 689, 756, 794, 812, 843, 912, 944, 953, 972, 1024, 1041, 1046, 1062, 1076, 1127, 1184, 1199, 1235, 1245, 1319, 1322, 1337, 1410, 1474, 1494, 1521, 1538, 1621, 1640, 1661, 1842, 2952, 3094, 3152, 3184, 3191, 3205, 3218, 3248

Rotational constants (GHZ): 1.30405 0.75704 0.52090

Zero-point correction= 0.153497 (Hartree/Particle)

Thermal correction to Energy= 0.163684

Thermal correction to Enthalpy= 0.164628

Thermal correction to Gibbs Free Energy= 0.116780

Sum of electronic and zero-point Energies= -572.967299

Sum of electronic and thermal Energies= -572.957112

Sum of electronic and thermal Enthalpies= -572.956168

Sum of electronic and thermal Free Energies= -573.004016

sCI_Indene1 (anti)

Frequencies: 41, 72, 113, 144, 190, 243, 254, 307, 315, 413, 435, 469, 514, 599, 608, 677, 753, 768, 798, 874, 911, 926, 987, 1001, 1023, 1047, 1048, 1065, 1097, 1153, 1199, 1214, 1221, 1236, 1318, 1321, 1346, 1453, 1462, 1497, 1498, 1531, 1621, 1647, 1673, 1838, 2953, 3085, 3144, 3186, 3191, 3203, 3206, 3216

Rotational constants (GHZ):   1.39877   0.64677   0.49170

Zero-point correction=   0.152875 (Hartree/Particle)//

Thermal correction to Energy=   0.163349

Thermal correction to Enthalpy=   0.164293

Thermal correction to Gibbs Free Energy=   0.115713

Sum of electronic and zero-point Energies=   -572.968926

Sum of electronic and thermal Energies=   -572.958452

Sum of electronic and thermal Enthalpies=   -572.957508

Sum of electronic and thermal Free Energies=   -573.006087

SO$_2$_sCI-Indene1 (SOZ)

Frequencies: 31, 39, 69, 104, 127, 183, 220, 254, 283, 329, 337, 390, 460, 468, 481, 504, 531, 579, 648, 652, 696, 714, 761, 767, 783, 825, 842, 868, 919, 959, 973, 1010, 1029, 1031, 1074, 1087, 1115, 1141, 1190, 1212, 1233, 1241, 1317, 1324, 1328, 1352, 1381, 1413, 1452, 1473, 1494, 1532, 1625, 1648, 1840, 3016, 3067, 3083, 3122, 3186, 3198, 3209, 3220

Rotational constants (GHZ):   0.83304   0.43446   0.38615

Zero-point correction=   0.165040 (Hartree/Particle)

Thermal correction to Energy=   0.177700

Thermal correction to Enthalpy=   0.178644

Thermal correction to Gibbs Free Energy=   0.124218

Sum of electronic and zero-point Energies=   -1121.530358

Sum of electronic and thermal Energies=   -1121.517698

Sum of electronic and thermal Enthalpies=   -1121.516753

Sum of electronic and thermal Free Energies=   -1121.571180

ST1_sCI-Indene1_aldhyde_SO$_3$

Frequencies: -626, 17, 39, 66, 101, 128, 158, 198, 211, 234, 272, 286, 399, 440, 455, 476, 489, 523, 529, 547, 615, 646, 719, 760, 778, 830, 844, 871, 924, 939, 962, 1012, 1033, 1057, 1060, 1063, 1109, 1177, 1191, 1213, 1231, 1239, 1296, 1314, 1326, 1352, 1375, 1430, 1460, 1491, 1522, 1536, 1624, 1644, 1842, 2995, 3048, 3091, 3156, 3184, 3193, 3207, 3216

Rotational constants (GHZ):   0.82141   0.42264   0.37208

Zero-point correction=   0.162085 (Hartree/Particle)

Thermal correction to Energy=   0.175205

Thermal correction to Enthalpy=   0.176149

Thermal correction to Gibbs Free Energy=   0.120101

Sum of electronic and zero-point Energies=   -1121.492295

Sum of electronic and thermal Energies=   -1121.479176

Sum of electronic and thermal Enthalpies=   -1121.478231

Sum of electronic and thermal Free Energies=   -1121.534279

ST2_sCI-Indene1_organic acid_SO₂

Frequencies: -921, 26, 47, 75, 95, 121, 156, 180, 249, 257, 278, 294, 344, 376, 452, 458, 478, 503, 518, 560, 604, 623, 648, 734, 765, 782, 824, 870, 905, 911, 918, 985, 997, 1023, 1034, 1036, 1071, 1120, 1189, 1206, 1217, 1239, 1265, 1283, 1308, 1322, 1339, 1388, 1460, 1488, 1500, 1533, 1624, 1647, 1843, 2513, 2998, 3070, 3126, 3176, 3191, 3204, 3219.

Rotational constants (GHZ):   1.08066   0.34276   0.29133

Zero-point correction=   0.158715 (Hartree/Particle)

Thermal correction to Energy=   0.172020

Thermal correction to Enthalpy=   0.172965

Thermal correction to Gibbs Free Energy=   0.117123

Sum of electronic and zero-point Energies=   -1121.482094

Sum of electronic and thermal Energies=   -1121.468789

Sum of electronic and thermal Enthalpies=   -1121.467845

Sum of electronic and thermal Free Energies=   -1121.523687

ST3_sCI-Indene1_ester_SO₂

Frequencies: -419, 27, 40, 72, 102, 109, 126, 182, 211, 259, 308, 338, 356, 428, 435, 472, 475, 488, 521, 535, 603, 619, 647, 734, 755, 790, 819, 847, 904, 918, 999, 1010, 1036, 1047, 1068, 1077, 1089, 1145, 1192, 1203, 1220, 1238, 1272, 1316, 1322, 1329, 1385, 1448, 1476, 1493, 1505, 1529, 1618, 1638, 1845, 3003, 3035, 3123, 3189, 3197, 3210, 3213, 3221

Rotational constants (GHZ):   0.82239   0.39335   0.35555

Zero-point correction=   0.161332 (Hartree/Particle)

Thermal correction to Energy=   0.174609

Thermal correction to Enthalpy=   0.175554

Thermal correction to Gibbs Free Energy=   0.119517

Sum of electronic and zero-point Energies=   -1121.489663

Sum of electronic and thermal Energies=   -1121.476386

Sum of electronic and thermal Enthalpies=   -1121.475442

Sum of electronic and thermal Free Energies=   -1121.531479

Aldehyde_Indene1 P1

Frequencies: 62, 100, 106, 135, 248, 262, 307, 366, 458, 472, 509, 522, 645, 690, 751, 764, 786, 832, 861, 908, 949, 996, 1039, 1041, 1063, 1066, 1123, 1179, 1207, 1225, 1235, 1309, 1315, 1364, 1433, 1481, 1489, 1518, 1535, 1626, 1645, 1842, 1882, 2931, 2999, 3040, 3079, 3176, 3189, 3200, 3213

Rotational constants (GHZ):   1.43890   1.06735   0.68975

Zero-point correction= 0.148483 (Hartree/Particle)

Thermal correction to Energy= 0.157953

Thermal correction to Enthalpy= 0.158897

Thermal correction to Gibbs Free Energy= 0.113080

Sum of electronic and zero-point Energies= -497.903648

Sum of electronic and thermal Energies= -497.894179

Sum of electronic and thermal Enthalpies= -497.893234

Sum of electronic and thermal Free Energies= -497.939051

Organic acid_Indene1 P2

Frequencies: 35, 63, 88, 122, 226, 243, 294, 312, 456, 460, 486, 513, 526, 613, 641, 649, 745, 771, 795, 830, 875, 906, 937, 971, 1010, 1045, 1067, 1078, 1109, 1156, 1189, 1210, 1233, 1246, 1311, 1320, 1330, 1401, 1446, 1494, 1526, 1535, 1623, 1646, 1836, 1882, 3018, 3105, 3162, 3186, 3197, 3208, 3217, 3846

Rotational constants (GHZ): 1.25025 0.80797 0.53605

Zero-point correction= 0.155357 (Hartree/Particle)

Thermal correction to Energy= 0.165588

Thermal correction to Enthalpy= 0.166532

Thermal correction to Gibbs Free Energy= 0.118133

Sum of electronic and zero-point Energies= -573.154235

Sum of electronic and thermal Energies= -573.144003

Sum of electronic and thermal Enthalpies= -573.143059

Sum of electronic and thermal Free Energies= -573.191459

Ester_Indene1 P3

Frequencies: 40, 58, 101, 141, 225, 232, 271, 307, 384, 398, 460, 472, 515, 625, 654, 750, 785, 794, 830, 855, 914, 955, 1000, 1021, 1036, 1058, 1067, 1070, 1126, 1181, 1212, 1224, 1239, 1296, 1313, 1350, 1420, 1431, 1478, 1489, 1530, 1551, 1626, 1647, 1838, 1854, 3058, 3089, 3111, 3172, 3174, 3188, 3200, 3212

Rotational constants (GHZ): 1.23975 0.83756 0.56310

Zero-point correction= 0.154980 (Hartree/Particle)

Thermal correction to Energy= 0.165245

Thermal correction to Enthalpy= 0.166190

Thermal correction to Gibbs Free Energy= 0.117882

Sum of electronic and zero-point Energies= -573.130742

Sum of electronic and thermal Energies= -573.120477

Sum of electronic and thermal Enthalpies= -573.119533

Sum of electronic and thermal Free Energies= -573.167840

Complex_sCI_Indene1(syn)-H$_2$O

Frequencies: 4, 68, 82, 114, 125, 178, 189, 199, 241, 260, 276, 334, 392, 421, 443, 467, 514, 528, 607, 678, 728, 741, 773, 795, 810, 879, 910, 925, 969, 992, 1009, 1048, 1050, 1057, 1078, 1146, 1197, 1213, 1227, 1242, 1326, 1332, 1363, 1419, 1462, 1492, 1496, 1531, 1617, 1648, 1659, 1685, 1824, 2958, 3057, 3119, 3179, 3191, 3204, 3211, 3225, 3556, 3984

Rotational constants (GHZ):   0.97615   0.70088   0.46964

Zero-point correction=   0.178719 (Hartree/Particle)

 Thermal correction to Energy=   0.191795

 Thermal correction to Enthalpy=   0.192739

 Thermal correction to Gibbs Free Energy=   0.136686

 Sum of electronic and zero-point Energies=   -649.385068

 Sum of electronic and thermal Energies=   -649.371992

 Sum of electronic and thermal Enthalpies=   -649.371048

 Sum of electronic and thermal Free Energies=   -649.427101

Complex_sCI_Indene1(anti)-H$_2$O

Frequencies: 25, 48, 55, 82, 107, 163, 182, 209, 238, 258, 277, 314, 350, 429, 453, 466, 508, 515, 595, 611, 676, 749 764, 786, 862, 876, 902, 912, 989, 994, 1031, 1035, 1048, 1065, 1090, 1147, 1188, 1210, 1220, 1242, 1311, 1319, 1339, 1379, 1488, 1515, 1524, 1619, 1643, 1685, 1776, 1845, 2952, 3110, 3174, 3181, 3189, 3194, 3200, 3213, 3619, 3996

 Rotational constants (GHZ):   1.30378   0.45246   0.36611

Zero-point correction=   0.178593 (Hartree/Particle)

 Thermal correction to Energy=   0.191954

 Thermal correction to Enthalpy=   0.192898

 Thermal correction to Gibbs Free Energy=   0.137021

 Sum of electronic and zero-point Energies=   -649.377978

 Sum of electronic and thermal Energies=   -649.364618

 Sum of electronic and thermal Enthalpies=   -649.363674

 Sum of electronic and thermal Free Energies=   -649.419551

ST_sCI_Indene1(syn)-H$_2$O

Frequencies: -451, 64, 80, 93, 142, 194, 227, 240, 269, 307, 371, 422, 435, 462, 507, 540, 591, 625, 639, 676, 699, 761, 776, 797, 884, 900, 926, 952, 1005, 1045,   1048, 1055, 1070, 1094, 1148, 1189, 1214, 1222, 1235, 1316, 1319, 1327, 1335, 1379, 1458, 1494, 1507, 1526, 1574, 1618, 1636, 1643, 1832, 2400, 2943, 3131, 3184, 3190, 3192, 3205, 3207, 3213, 3923

Rotational constants (GHZ):   1.22652   0.59715   0.43647

Zero-point correction=   0.178749 (Hartree/Particle)

Thermal correction to Energy= 0.190092

Thermal correction to Enthalpy= 0.191036

Thermal correction to Gibbs Free Energy= 0.141165

Sum of electronic and zero-point Energies= -649.362125

Sum of electronic and thermal Energies= -649.350782

Sum of electronic and thermal Enthalpies= -649.349838

Sum of electronic and thermal Free Energies= -649.399709

ST_sCI_Indene1(anti)-H$_2$O

Frequencies: -437, 38, 64, 69, 122, 191, 230, 237, 273, 291, 382, 411, 435, 457, 500, 517, 566, 593, 638, 679, 687, 754, 779, 800, 874, 900, 921, 991, 1004, 1042, 1047, 1056, 1082, 1144, 1181, 1192, 1213, 1220, 1234, 1316, 1320, 1330, 1352, 1409, 1449, 1488, 1494, 1530, 1593, 1619, 1633, 1647, 1841, 2299, 2949, 3096, 3159, 3183, 3190, 3202, 3213, 3220, 3925

Rotational constants (GHZ): 1.28304 0.51781 0.41543

Zero-point correction= 0.178328 (Hartree/Particle)

Thermal correction to Energy= 0.189910

Thermal correction to Enthalpy= 0.190854

Thermal correction to Gibbs Free Energy= 0.139671

Sum of electronic and zero-point Energies= -649.362987

Sum of electronic and thermal Energies= -649.351406

Sum of electronic and thermal Enthalpies= -649.350462

Sum of electronic and thermal Free Energies= -649.401645

Product_sCI_Indene1(anti)-H$_2$O

Frequencies: 51, 62, 70, 111, 161, 194, 226, 278, 290, 309, 362, 374, 418, 441, 466, 506, 563, 614, 647, 676, 758, 781, 793, 860, 901, 920, 999, 1029, 1034, 1041, 1051, 1071, 1084, 1123, 1148, 1193, 1208, 1222, 1228, 1298, 1316, 1340, 1375, 1389, 1449, 1457, 1464, 1475, 1499, 1531, 1619, 1649, 1839, 2931, 3062, 3121, 3142, 3181, 3191, 3202, 3212, 3826, 3907

Rotational constants (GHZ): 1.17262 0.57903 0.44913

Zero-point correction= 0.181669 (Hartree/Particle)

Thermal correction to Energy= 0.193800

Thermal correction to Enthalpy= 0.194744

Thermal correction to Gibbs Free Energy= 0.142716

Sum of electronic and zero-point Energies= -649.431719

Sum of electronic and thermal Energies= -649.419588

Sum of electronic and thermal Enthalpies= -649.418644

Sum of electronic and thermal Free Energies=   -649.470672

Indne 2

ST_Indene2OOO_cyclic_sCI-Indene2

Frequencies: -423, 105, 115, 217, 251, 334, 388, 433, 447, 473, 505, 555, 592, 619, 641, 673, 749, 777, 824, 883, 897, 918, 954, 986, 1023, 1043, 1059, 1113, 1135, 1184, 1187, 1207, 1225, 1250, 1258, 1289, 1304, 1335, 1353, 1412, 1483, 1506, 1514, 1522, 1625, 1651, 2954, 3063, 3110, 3170, 3181, 3188, 3198, 3211

Rotational constants (GHZ):   2.26818   0.70190   0.57717

Zero-point correction=   0.152849 (Hartree/Particle)

Thermal correction to Energy=   0.161409

Thermal correction to Enthalpy=   0.162354

Thermal correction to Gibbs Free Energy=   0.119045

Sum of electronic and zero-point Energies=   -572.917895

Sum of electronic and thermal Energies=   -572.909335

Sum of electronic and thermal Enthalpies=   -572.908391

Sum of electronic and thermal Free Energies=   -572.951699

sCI_Indene2_(syn)

Frequencies: 47, 53, 101, 154, 166, 239, 287, 318, 413, 421, 444, 516, 527, 581, 612, 703, 761, 784, 795, 860, 873, 909, 937, 984, 1008, 1040, 1040, 1061, 1069, 1124, 1188, 1203, 1206, 1242, 1295, 1322, 1337, 1474, 1485, 1491, 1503, 1576, 1598, 1634, 1643, 1886, 2918, 3055, 3140, 3186, 3199, 3212, 3214, 3259

Rotational constants (GHZ):   1.13572   0.75859   0.48350

Zero-point correction=   0.152854 (Hartree/Particle)

Thermal correction to Energy=   0.163207

Thermal correction to Enthalpy=   0.164151

Thermal correction to Gibbs Free Energy=   0.115622

Sum of electronic and zero-point Energies=   -572.967034

Sum of electronic and thermal Energies=   -572.956682

Sum of electronic and thermal Enthalpies=   -572.955737

Sum of electronic and thermal Free Energies=   -573.004266

sCI_Indene2 (anti)

Frequencies: 48, 79, 89, 143, 161, 175, 256, 321, 341, 401, 479, 486, 502, 536, 598, 647, 757, 785, 795, 849, 897, 905, 993, 1004, 1005, 1033, 1039, 1066, 1075, 1133, 1187, 1199, 1215, 1262, 1300, 1318, 1332, 1421, 1460, 1493, 1519, 1562, 1604, 1629, 1651, 1883, 2883, 3072, 3137, 3172, 3188, 3198, 3208, 3218

Rotational constants (GHZ):   0.97998   0.79689   0.46497

Zero-point correction=   0.151979 (Hartree/Particle)

Thermal correction to Energy=   0.162617

Thermal correction to Enthalpy=   0.163562

Thermal correction to Gibbs Free Energy=   0.114515

Sum of electronic and zero-point Energies=   -572.967884

Sum of electronic and thermal Energies=   -572.957245

Sum of electronic and thermal Enthalpies=   -572.956301

Sum of electronic and thermal Free Energies=   -573.005348

SO$_2$_ sCI-Indene2 (SOZ)

Frequencies: 38, 45, 84, 90, 121, 141, 179, 235, 267, 297, 339, 364, 445, 452, 479, 488, 533, 544, 594, 653, 666, 711, 760, 778, 788, 794, 859, 892, 926, 939, 1000, 1019, 1034, 1039, 1072, 1078, 1107, 1161, 1187, 1208, 1220, 1270, 1300, 1302, 1323, 1343, 1401, 1458, 1470, 1491, 1512, 1540, 1628, 1651, 1874, 3004, 3075, 3082, 3133, 3181, 3193, 3205, 3217

Rotational constants (GHZ):   0.79231   0.41663   0.28847

Zero-point correction=   0.164670 (Hartree/Particle)

Thermal correction to Energy=   0.177648

Thermal correction to Enthalpy=   0.178592

Thermal correction to Gibbs Free Energy=   0.123514

Sum of electronic and zero-point Energies=   -1121.523743

Sum of electronic and thermal Energies=   -1121.510765

Sum of electronic and thermal Enthalpies=   -1121.509820

Sum of electronic and thermal Free Energies=   -1121.564899

ST1_ Indene2_aldehyde_SO$_3$

Frequencies: -623, 51, 55, 76, 110, 119, 164, 176, 217, 242, 327, 344, 370, 441, 467, 486, 525, 541, 555, 586, 595, 637, 709, 777, 785, 811, 844, 885, 920, 929, 1003, 1028, 1037, 1040, 1077, 1084, 1122, 1138, 1194, 1205, 1215, 1227, 1248, 1304, 1326, 1338, 1350, 1411, 1477, 1495, 1536, 1545, 1628, 1654, 1876, 2989, 3028, 3087, 3141, 3177, 3191, 3203, 3217

Rotational constants (GHZ):   0.77475   0.42680   0.30603

Zero-point correction=   0.162521 (Hartree/Particle)

Thermal correction to Energy=   0.175322

Thermal correction to Enthalpy=   0.176266

Thermal correction to Gibbs Free Energy=   0.121955

Sum of electronic and zero-point Energies=   -1121.490407

Sum of electronic and thermal Energies=   -1121.477605

Sum of electronic and thermal Enthalpies=   -1121.476661

Sum of electronic and thermal Free Energies=   -1121.530972

ST2_ Indene2_organic acid_SO₂

Frequencies: -925, 41, 45, 58, 103, 114, 175, 182, 208, 239, 276, 313, 344, 411, 439, 467, 474, 521, 532, 552, 577, 598, 661, 746, 775, 788, 823, 842, 875, 897, 922, 1002, 1031, 1039, 1043, 1071, 1074, 1108, 1162, 1188, 1211, 1221, 1304, 1309, 1322, 1329, 1340, 1366, 1489, 1494, 1500, 1526, 1622, 1642, 1873, 2505, 2994, 3082, 3142, 3181, 3193, 3204, 3217

Rotational constants (GHZ):   0.75892   0.42763   0.30669

Zero-point correction=   0.158983 (Hartree/Particle)

Thermal correction to Energy=   0.172292

Thermal correction to Enthalpy=   0.173236

Thermal correction to Gibbs Free Energy=   0.117518

Sum of electronic and zero-point Energies=   -1121.484559

Sum of electronic and thermal Energies=   -1121.471249

Sum of electronic and thermal Enthalpies=   -1121.470305

Sum of electronic and thermal Free Energies=   -1121.526024

ST3_ Indene2_ester_SO₂

Frequencies: -536, 34, 64, 79, 87, 117, 148, 182, 230, 250, 318, 325, 388, 415, 437, 478, 481, 507, 547, 589, 600, 657, 716, 741, 768, 792, 836, 895, 906, 985, 1000, 1027, 1034, 1047, 1062, 1075, 1149, 1156, 1194, 1210, 1226, 1260, 1276, 1295, 1307, 1334, 1342, 1443, 1449, 1475, 1511, 1528, 1598, 1627, 1869, 3027, 3076, 3094, 3156, 3188, 3200, 3206, 3220

Rotational constants (GHZ):   0.85197   0.41194   0.30867

Zero-point correction=   0.162285 (Hartree/Particle)

Thermal correction to Energy=   0.175261

Thermal correction to Enthalpy=   0.176205

Thermal correction to Gibbs Free Energy=   0.121290

Sum of electronic and zero-point Energies=   -1121.484757

Sum of electronic and thermal Energies=   -1121.471781

Sum of electronic and thermal Enthalpies=   -1121.470837

Sum of electronic and thermal Free Energies=   -1121.525752

Aldehyde_Indene2 P1

Frequencies: 43, 78, 116, 169, 248, 258, 312, 371, 452, 469, 496, 543, 603, 651, 759, 785, 808, 828, 880, 928, 1015, 1028, 1050, 1060, 1067, 1073, 1127, 1185, 1198, 1213, 1238, 1294, 1312, 1331, 1463, 1491, 1496, 1523, 1556, 1621, 1646, 1838, 1880, 2923, 2972, 3076, 3139, 3186, 3196, 3206, 3219

Rotational constants (GHZ):   1.42050   0.92337   0.60068

Zero-point correction=   0.149039 (Hartree/Particle)

Thermal correction to Energy=   0.158509

Thermal correction to Enthalpy=   0.159453

Thermal correction to Gibbs Free Energy=   0.113205

Sum of electronic and zero-point Energies=   -497.902728

Sum of electronic and thermal Energies=   -497.893258

Sum of electronic and thermal Enthalpies=   -497.892313

Sum of electronic and thermal Free Energies=   -497.938562

Organic acid_Indene2 P2

Frequencies: 44, 54, 102, 149, 252, 276, 296, 368, 418, 441, 453, 534, 553, 624, 641, 655, 742, 762, 781, 829, 839, 877, 921, 1009, 1034, 1037, 1062, 1083, 1126, 1152, 1196, 1219, 1224, 1234, 1304, 1313, 1347, 1398, 1445, 1493, 1532, 1565, 1617, 1651, 18533, 1877, 2945, 3099, 3147, 3180, 3195, 3207, 3229, 3846

Rotational constants (GHZ):   1.22434   0.84168   0.52701

Zero-point correction=   0.155447 (Hartree/Particle)

Thermal correction to Energy=   0.165504

Thermal correction to Enthalpy=   0.166448

Thermal correction to Gibbs Free Energy=   0.118679

Sum of electronic and zero-point Energies=   -573.151284

Sum of electronic and thermal Energies=   -573.141227

Sum of electronic and thermal Enthalpies=   -573.140282

Sum of electronic and thermal Free Energies=   -573.188052

Ester_Indene2 P3

Frequencies:43, 73, 100, 126, 139, 182, 275, 296, 342, 421, 468, 494, 525, 577, 605, 674, 759, 789, 799, 859, 904, 911, 993, 1021, 1032, 1068, 1069, 1076, 1132, 1173, 1181, 1207, 1216, 1281, 1303, 1311, 1337, 1441, 1476, 1484, 1493, 1534, 1631, 1649, 1874, 1908, 2959, 3038, 3066, 3141, 3188, 3194, 3203, 3214

Rotational constants (GHZ):   0.98029   0.85281   0.48600

Zero-point correction=   0.153227 (Hartree/Particle)

Thermal correction to Energy=   0.163820

Thermal correction to Enthalpy=   0.164764

Thermal correction to Gibbs Free Energy=   0.115641

Sum of electronic and zero-point Energies=   -573.127834

Sum of electronic and thermal Energies=   -573.117241

Sum of electronic and thermal Enthalpies=   -573.116297

Sum of electronic and thermal Free Energies=   -573.165419

Complex_sCI_Indene2(syn)-H₂O

Frequencies: 29, 46, 67, 92, 129, 161, 175, 194, 195, 233, 278, 315, 404, 415, 445, 505, 512, 538, 575, 606, 670, 704, 765, 785, 802, 860, 872, 919, 950, 960, 1022, 1026, 1050, 1062, 1069, 1123, 1197, 1202, 1214, 1245, 1300, 1326, 1339, 1454, 1469, 1492, 1511, 1531, 1606, 1632, 1649, 1711, 1884, 2916, 3066, 3136, 3189, 3203, 3214, 3219, 3255, 3700, 3986

Rotational constants (GHZ):   0.98437   0.54673   0.41428

Zero-point correction=   0.178163 (Hartree/Particle)

Thermal correction to Energy=   0.191561

Thermal correction to Enthalpy=   0.192506

Thermal correction to Gibbs Free Energy=   0.136877

Sum of electronic and zero-point Energies=   -649.374009

Sum of electronic and thermal Energies=   -649.360611

Sum of electronic and thermal Enthalpies=   -649.359667

Sum of electronic and thermal Free Energies=   -649.415295

Complex_sCI_Indene2(anti)-H₂O

Frequencies: 25, 48, 55, 82, 107, 163, 182, 209, 238, 258, 277, 314, 350, 429, 453, 466, 508, 515, 595, 611, 676, 749, 764, 786, 862, 876, 902, 912, 989, 994, 1031, 1035, 1048, 1065, 1090, 1147, 1188, 1210, 1220, 1242, 1311, 1319, 1339, 1379, 1446, 1488, 1515, 1524, 1619, 1643, 1685, 1776, 1845, 2952, 3110, 3174, 3181, 3189, 3194, 3200, 3213, 3619, 3996

Rotational constants (GHZ):   1.30378   0.45246   0.36611

Zero-point correction=   0.178593 (Hartree/Particle)

Thermal correction to Energy=   0.191954

Thermal correction to Enthalpy=   0.192898

Thermal correction to Gibbs Free Energy=   0.137021

Sum of electronic and zero-point Energies=   -649.377978

Sum of electronic and thermal Energies=   -649.364618

Sum of electronic and thermal Enthalpies=   -649.363674

Sum of electronic and thermal Free Energies=   -649.419551

ST_sCI_Indene2(syn)-H₂O

Frequencies: -601, 43, 65, 92, 109, 140, 181, 247, 294, 321, 343, 396, 440, 470, 521, 536, 555, 602, 634, 684, 725, 768, 792, 797, 861, 874, 913, 937, 1020, 1036, 1049, 1066, 1067, 1074, 1119, 1137, 1187, 1205, 1220, 1242, 1310, 1324, 1336, 1418, 1442, 1487, 1513, 1541, 1560, 1617, 1642, 1653, 1881, 2122, 2917, 3070, 3135, 3180, 3184, 3196, 3206, 3233, 3924

Rotational constants (GHZ):   0.99789   0.63050   0.44051

Zero-point correction=   0.176916 (Hartree/Particle)

Thermal correction to Energy=   0.188582

Thermal correction to Enthalpy=   0.189526

Thermal correction to Gibbs Free Energy=   0.138255

Sum of electronic and zero-point Energies=   -649.351055

Sum of electronic and thermal Energies=   -649.339389

Sum of electronic and thermal Enthalpies=   -649.338445

Sum of electronic and thermal Free Energies=   -649.389716

ST_sCI_Indene2(anti)-H₂O

Frequencies:-437, 38, 64, 69, 122, 191, 230, 237, 273, 291, 382, 411, 435, 457, 500, 517, 566, 593, 638, 679, 687, 754, 779, 800, 874, 900, 921, 991, 1004, 1042, 1047, 1056, 1082, 1144, 1181, 1192, 1213, 1220, 1234, 1316, 1320, 1330, 1352, 1409, 1449, 1488, 1494, 1530, 1593, 1619, 1633,   1647, 1841, 2299, 2949, 3096, 3159, 3183, 3190, 3202, 3213, 3220, 3925

Rotational constants (GHZ):   1.28304   0.51781   0.41543

Zero-point correction=   0.178328 (Hartree/Particle)

 Thermal correction to Energy=   0.189910

 Thermal correction to Enthalpy=   0.190854

 Thermal correction to Gibbs Free Energy=   0.139671

 Sum of electronic and zero-point Energies=   -649.362987

 Sum of electronic and thermal Energies=   -649.351406

 Sum of electronic and thermal Enthalpies=   -649.350462

 Sum of electronic and thermal Free Energies=   -649.401645

Product_sCI_Indene2_H₂O

 Frequencies: 90, 104, 116, 152, 174, 189, 246, 257, 303, 323, 357, 410, 431, 476, 494, 515, 572, 651, 667, 696, 758, 783, 798, 849. 886, 911, 955, 995, 1017, 1037, 1048, 1070, 1074, 1112, 1140, 1185, 1208, 1228, 1250, 1300, 1310, 1338, 1368, 1427, 1449, 1451, 1485, 1497, 1533, 1619, 1650, 1653, 1868, 2944, 3026, 3086, 3106, 3179, 3191, 3202, 3218, 3821

 Rotational constants (GHZ):   0.98895   0.71963   0.48990

 Zero-point correction=   0.182664 (Hartree/Particle)

 Thermal correction to Energy=   0.194297

 Thermal correction to Enthalpy=   0.195241

 Thermal correction to Gibbs Free Energy=   0.145377

 Sum of electronic and zero-point Energies=   -649.424054

 Sum of electronic and thermal Energies=   -649.412421

 Sum of electronic and thermal Enthalpies=   -649.411477

 Sum of electronic and thermal Free Energies=   -649.461341