

**How Well Can Theory Predict Addition-Fragmentation Equilibrium Constants in RAFT
Polymerisation?**

Ching Yeh Lin and Michelle L. Coote¹

ARC Centre of Excellence for Free-Radical Chemistry and Biotechnology, Research School of
Chemistry, Australian National University, Canberra ACT 0200, Australia

SUPPORTING INFORMATION

¹ Correspondence to mcoote@rsc.anu.edu.au

Table S1. Absolute entropies (S in J/mol K), temperature corrections (TC in Hartrees) and zero-point vibrational energies (ZPVE in Hartrees) at B3-LYP/6-31G(d) optimized geometries level of theory; absolute energies (E), enthalpies (H), Gibbs free energies in gas phase (G_{gas}) and in toluene (G_{soln}) all in Hartrees at W1-ONIOM for the species in this study at 243.15K.

	S	TC	ZPVE	E	H	G_{gas}	G_{soln}
n.SM2	608.27850	0.01541	0.22420	-1845.69486	-1845.88824	-1845.94458	-1845.95342
r.M	334.00890	0.00617	0.10325	-306.58324	-306.63782	-306.66875	-306.67420
r.I1	382.82660	0.00754	0.12438	-781.31013	-781.41751	-781.45297	-781.46016
r.I1M	520.84170	0.01248	0.22227	-1087.19878	-1087.36334	-1087.41157	-1087.42082
r.I1MM	671.04700	0.01782	0.32008	-1393.12769	-1393.34912	-1393.41127	-1393.42400
r.I2	376.53520	0.00758	0.20282	-404.39257	-404.43088	-404.46576	-404.47411
r.I2M	496.55390	0.01205	0.30139	-710.26364	-710.35893	-710.40491	-710.41546
r.I2MM	637.22100	0.01716	0.40012	-1016.19283	-1016.34430	-1016.40331	-1016.41351
r.MMM	604.49680	0.01594	0.30129	-918.44432	-918.61112	-918.66711	-918.67394
r.SM3	731.42030	0.02095	0.33244	-2152.31875	-2152.56234	-2152.63008	-2152.63269
r.SI1SM2	772.86030	0.02244	0.35242	-2627.05791	-2627.35534	-2627.42692	-2627.43186
r.SMI1SM2	916.00820	0.02759	0.45028	-2932.93601	-2933.29044	-2933.37528	-2933.38178
r.SMMI1SM2	1056.52480	0.03283	0.54880	-3238.87014	-3239.28085	-3239.37869	-3239.38271
r.SI2SM2	753.05250	0.02222	0.43151	-2250.13063	-2250.35860	-2250.42834	-2250.43354
r.SMI2SM2	888.75400	0.02709	0.53010	-2556.00034	-2556.28487	-2556.36717	-2556.37229
r.SMMI2SM2	1018.10710	0.03210	0.62880	-2861.93303	-2862.27388	-2862.36817	-2862.37146
r.SMMMSM2	994.09880	0.03094	0.53004	-2764.18229	-2764.53833	-2764.63040	-2764.63156
r.M(core=CH3)	334.00890	0.00617	0.10325	-306.53184	-306.58642	-306.61735	-306.62280
n.S=CSI1SM	644.46390	0.01689	0.24384	-2320.47423	-2320.72180	-2320.78148	-2320.79375
n.S=CSMI1SM	790.02680	0.02201	0.34210	-2626.36245	-2626.66666	-2626.73983	-2626.75299
n.S=CSMMI1SM	926.66530	0.02723	0.44067	-2932.29480	-2932.65524	-2932.74106	-2932.75378
n.S=CSI2SM	630.39450	0.01681	0.32311	-1943.55342	-1943.73121	-1943.78959	-1943.80230
n.S=CSMI2SM	769.14710	0.02153	0.42195	-2249.42656	-2249.66081	-2249.73204	-2249.74355
n.S=CSMMI2SM	889.44290	0.02652	0.52067	-2555.35742	-2555.64799	-2555.73036	-2555.74166
n.S=CSMMMSM	884.41500	0.02568	0.42141	-2457.60750	-2457.91344	-2457.99535	-2458.00459

Table S2. Relative temperature *entropies (ΔTS) at B3-LYP/6-31G(d) optimized geometries level of theory and relative enthalpies (ΔH), Gibbs free energies in gas phase (ΔG_{gas}) and in toluene (ΔG_{soln}) all in kJ/mol and their corresponding equilibrium constants $K(\text{L/mol})$ at W1-ONIOM for the reactions in this study at 243.15K.

		ΔTS	ΔH	ΔG_{gas}	ΔG_{soln}	K_{gas}	K_{soln}
	rn(1)	-51.27	-95.24	-43.97	-19.36	5.6E+10	1.4E+04
I=I1	rn(2)	-53.07	-130.18	-77.11	-54.04	7.3E+17	4.1E+11
	rn(3)	-51.82	-102.03	-50.21	-25.85	1.2E+12	3.6E+05
	rn(4)	-54.17	-114.16	-59.99	-19.93	1.5E+14	1.9E+04
I=I2	rn(2)	-56.35	-103.64	-47.29	-21.83	2.9E+11	4.9E+04
	rn(3)	-52.54	-98.97	-46.43	-14.99	1.9E+11	1.7E+03
	rn(4)	-55.29	-108.52	-53.23	-17.95	5.4E+12	7.2E+03
no I	rn(5)	-53.17	-102.30	-49.13	-17.06	7.1E+11	4.6E+03
I=I1	rn(6)	-49.99	-123.72	-73.72	-46.22	1.4E+17	8.5E+09
	rn(7)	-50.58	-98.09	-47.51	-21.76	3.2E+11	4.7E+04
	rn(8)	-49.64	-102.88	-53.24	-22.13	5.4E+12	5.7E+04
I=I2	rn(6)	-51.39	-107.58	-56.19	-28.18	2.3E+13	1.1E+06
	rn(7)	-52.13	-98.80	-46.67	-21.64	2.1E+11	4.4E+04
	rn(8)	-49.93	-103.63	-53.70	-24.44	6.9E+12	1.8E+05
no I	rn(9)	-54.54	-101.00	-46.45	-16.98	1.9E+11	4.4E+03
I=I1	rn(10)	-3.07	-6.46	-3.39	-7.82	5.3E+00	4.8E+01
	rn(11)	-1.24	-3.94	-2.70	-4.08	3.8E+00	7.5E+00
	rn(12)	-4.54	-11.29	-6.75	2.20	2.8E+01	3.4E-01
I=I2	rn(10)	-4.96	3.94	8.90	6.35	1.2E-02	4.3E-02
	rn(11)	-0.41	-0.16	0.24	6.65	8.9E-01	3.7E-02
	rn(12)	-5.36	-4.89	0.47	6.49	7.9E-01	4.0E-02
no I	rn(13)	1.37	-1.31	-2.68	-0.08	3.8E+00	1.0E+00

Table S3. Complete B3-LYP/6-31G(d) Optimized Geometries

n.S=CSI1SM

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1\1\GINC-X2\FOpt\RB3LYP\Gen\C13H14O3S4\CYL509\02-Mar-2009\0\#\B3LYP/ge
n 6D INT(grid=ultrafine) OPT maxdisk=1342177280\ \n.S=CSI1SM.a4.freq\ \0
,C,-0.1026694975,-0.3559890251,0.3962225408\S,0.0022634278,-0.022863
7255,2.1148215417\C,1.8215840318,-0.0240312692,2.3951389523\C,2.061035
5284,0.5701772638,3.7965879727\H,2.2808661727,0.6160051495,1.638677582
7\C,2.5279275117,-1.3767211645,2.2901143968\O,3.7317703263,-1.45829792
72,2.1863001685\O,1.7044548296,-2.430169633,2.4080748914\C,2.342999730
3,-3.7170183062,2.3370560572\H,1.5404787594,-4.4458776361,2.450319765\
H,3.0795255622,-3.8233352274,3.1376597104\H,2.8415552984,-3.8380700999
,1.3720982785\S,1.1659144808,-0.6105618557,-0.6333138653\S,-1.70640402
98,-0.4435132091,-0.3887715972\C,-3.023261998,-0.1486480905,0.86082306
89\O,-2.7779483221,0.1715780827,2.0045522568\C,-4.403263011,-0.3051291
075,0.3347088789\C,-7.0826698101,-0.5339852713,-0.5099426677\C,-5.4584
113368,0.092392232,1.1776412959\C,-4.7126374976,-0.8241835324,-0.93036
38004\C,-6.034834798,-0.9384771002,-1.3504900862\C,-6.7748371161,-0.01
66523891,0.7637938927\H,-5.2197396609,0.4892960659,2.1585598552\H,-3.9
266456921,-1.1583562309,-1.6002995437\H,-6.2372465263,-1.348197486,-2.
3331581485\H,-7.576846532,0.2990761647,1.4255040181\S,-8.8023391838,-0
.6275514805,-0.9302852242\C,-8.8034020659,-1.3169684181,-2.6178784066\
H,-8.2832960159,-0.6605347999,-3.3203699287\H,-9.8554582058,-1.3799373
671,-2.9063624349\H,-8.3699702576,-2.320186668,-2.6430821957\H,3.13808
87251,0.5926833614,3.9864254296\H,1.672116466,1.5905864456,3.857774470
2\H,1.5840225684,-0.0321899775,4.5769264635\ \Version=EM64L-G03RevE.01\
State=1-A\HF=-2322.2432152\RMSD=5.864e-09\RMSF=2.017e-05\Thermal=0.\Di
pole=-1.8826803,-0.5615574,-0.2552712\PG=C01 [X(C13H14O3S4)]\@
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n.S=CSMI1SM

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\C,8.8369000322,1.6163549478,2.9473582791\S,8.4031847786,0.5047329554,
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8565376496,1.9973318055\C,10.0277156956,0.1028129492,5.0650675388\C,7.
8240261888,3.1853803852,0.8125938116\C,7.6338701321,2.7440928824,-0.63
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80170294,0.9970469528\C,7.1204142149,4.5172265139,1.0748170409\O,6.824
3216312,5.2885978632,0.1870969975\O,6.9532269978,4.7682544605,2.379718
3019\C,6.3481715494,6.0355907588,2.6920850031\H,6.282294899,6.06419924
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,9.2801384872,-3.8670975493,4.8035426625\H,10.9274117009,-3.8498918493
,5.4796437312\H,11.2654304614,0.7267713081,6.7193446306\H,10.299472449
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1.0610196219,-7.6706290237\S,4.3871869476,0.96222357,-6.590429794\H,5.
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487098797\C,4.0757981119,1.4151535517,-3.9334889786\H,3.036341699,1.16
85004859,-4.1329666307\H,7.0924382712,1.7173545639,-5.5032162436\H,7.7
804769516,2.2967620176,-3.2395289958\H,3.7568381103,1.7577831483,-1.83
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n.S=CSMMI1SM

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n.S=CSMI2SM

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P/gen 6D INT(grid=ultrafine) OPT maxdisk=1342177280\ \n.S=CSMI2SM.freq\
\0,1\C,8.9832699534,-5.9946180669,0.997330245\S,9.3232228722,-7.551677
7782,1.7857310675\S,7.7732820539,-4.9426003959,1.377584996\S,10.205170
1176,-5.8071799136,-0.2785860519\C,8.0807303387,-7.6317968755,3.160822
1077\C,9.7545709644,-4.2103151139,-1.1194443719\C,10.6638547293,-3.068
8939353,-0.6344441671\C,6.8245643974,-8.3946529954,2.7493406272\H,8.69
9949389,-4.0504857734,-0.8886843218\C,9.922360438,-4.525206193,-2.6028
262865\O,10.9839021897,-4.5260311812,-3.1886133914\O,8.7417943423,-4.8
265654807,-3.172920643\C,8.8040295279,-5.2000392067,-4.562434111\H,7.7
748705381,-5.4115710182,-4.8520396949\H,9.4317432398,-6.0855671074,-4.
6894903369\H,9.2136293276,-4.3810641128,-5.1589697285\H,7.8599561577,-
6.5920373051,3.4135570173\C,8.8022005906,-8.2981244624,4.329098856\O,8.
.8149020404,-9.4913030002,4.5376014706\O,9.426057044,-7.3857165189,5.0
959978786\C,10.1794129934,-7.9188901395,6.2005811154\H,10.6110917529,-
7.0530031313,6.7023148904\H,10.9649735015,-8.5868607174,5.8380721769\H
,9.5238123712,-8.4718560865,6.8780523283\H,6.1080307787,-8.3983002527,
3.5791958178\H,6.3540289136,-7.9119292631,1.8892865275\H,7.0630630834,
-9.4316125379,2.5017405717\H,10.7517846056,-3.1282933597,0.454093745\H
,11.657998664,-3.2616994561,-1.0441062677\O,13.4314583217,1.2497791876
, -0.5507680892\C,12.3049896278,1.328597549,0.308403381\C,11.0669280521
,0.66609128,-0.2999427185\N,11.3611183301,-0.739433824,-0.5987688252\C
,12.504388693,-0.7801019427,-1.5207634172\C,13.7121691438,-0.104673092
4,-0.8741843328\C,10.2066333934,-1.6134891006,-0.9759173905\C,8.989753
9296,-1.2828133473,-0.0913849585\C,9.7982033437,-1.4442469678,-2.45756
55954\H,8.8868190632,-2.0102030917,-2.682878664\H,10.5794533214,-1.779
4995951,-3.1450465734\H,9.5836749119,-0.3910132565,-2.6719800282\H,9.2
698876306,-1.2546577507,0.9671304321\H,8.2181549069,-2.0491855277,-0.2
069952151\H,8.5338760565,-0.324792494,-0.3604661052\H,14.0032104424,-0
.6609912759,0.0321652664\H,12.53025386,0.8461379992,1.274202979\H,10.7
639956556,1.2370005399,-1.1993798945\H,12.2890509045,-0.260302699,-2.4
723050778\H,14.5595730983,-0.088482042,-1.5667696402\H,12.1204295319,2
.3937553236,0.4810831416\H,10.2581498334,0.7379504042,0.4301154063\H,1
2.7645460321,-1.8139248974,-1.7647161469\Version=EM64L-G03RevE.01\Sta
te=1-A\HF=-2251.3809879\RMSD=8.388e-09\RMSF=1.147e-06\Thermal=0.\Dipol
e=-0.7792732,0.0994043,0.0639664\PG=C01 [X(C16H27N1O5S3)]\@

n.S=CSMMI2SM

1\1\GINC-X13\FOpt\RB3LYP\Gen\C20H33N1O7S3\CYL509\10-Mar-2009\0\#\B3LYP
/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1342177280\ \n.S=CS
MMI2SM.freq\0,1\O,12.7594558907,2.7174764364,-0.0602906024\C,14.08362
79669,2.9631737915,0.3861629082\C,14.6567550749,1.7827656599,1.1737055

48\N,14.6357067747,0.5795404581,0.3359781698\C,13.2450167941,0.3325861316,-0.0683891328\C,12.7140992655,1.5346147669,-0.8465359979\C,15.3741591277,-0.6205907371,0.8427463866\C,16.7183574109,-0.1788214541,1.4532676948\C,15.6871617212,-1.487552221,-0.4158456008\C,16.2633477022,-2.9010125846,-0.1764115583\C,15.1425862927,-3.8843367573,0.1439008094\O,15.5499812441,-4.8262893589,1.0293583418\C,14.5712531609,-5.8371841521,1.3332276172\O,14.0280532785,-3.857075431,-0.3294982397\C,14.5746529284,-1.3931066305,1.9173034012\H,13.67259227,-5.3825843543,1.7574157195\H,15.0479899577,-6.4948784876,2.061074423\H,14.3039143792,-6.3843678336,0.4259151271\H,14.7874628039,-1.6137119528,-1.0222392871\H,16.3931348818,-0.9093228146,-1.021995301\H,15.1696599208,-2.2099319516,2.3418076802\H,13.6547491348,-1.8258674734,1.5154115359\H,14.3062302532,-0.7255967682,2.7444033059\H,17.254077283,0.4944976575,0.7749074655\H,17.355509379,-1.0505428956,1.631291973\H,16.5920918582,0.3231631674,2.4176992559\H,13.3050907685,1.6667508303,-1.7679679177\H,14.7414390227,3.1711200289,-0.4744323974\H,14.0727615958,1.6617294115,2.1071314377\H,12.5827575783,0.1680681055,0.8014512426\H,11.6644645531,1.3839798295,-1.1180051101\H,14.0371730807,3.8561463865,1.0179305709\H,15.6823711262,2.0350034322,1.4516075753\H,13.1811744025,-0.5574080507,-0.7001475796\H,16.9630646939,-2.9024210186,0.666216583\C,20.6013214416,-3.8610221987,-1.9907801124\S,21.9068156726,-4.1391372258,-3.1618794591\S,20.682070795,-2.9526316947,-0.6176607211\S,19.1881275321,-4.7556673191,-2.5890611276\C,23.2608693382,-3.0045000737,-2.5934458668\C,17.9532570422,-4.5922317233,-1.2108656791\C,17.0476411283,-3.3725030802,-1.434479732\C,24.2787738934,-3.7301579779,-1.7178630992\H,18.5465482363,-4.4887045941,-0.2986459372\C,17.2224604981,-5.9325013043,-1.1904348475\O,16.1842264843,-6.1603188974,-1.7727661226\O,17.9078039841,-6.8402390083,-0.4744826704\C,17.3639896973,-8.1718929601,-0.4737555981\H,18.0694071674,-8.7728582473,0.0999557263\H,17.2762996247,-8.548830113,-1.4958416034\H,16.378032172,-8.1828006283,-0.0023827723\H,22.7580254152,-2.2011129804,-2.0501587718\C,23.891042907,-2.4449137151,-3.8659050448\O,24.8215217734,-2.9532581646,-4.4515801947\O,23.2734749052,-1.3148088877,-4.2543885078\C,23.7628577854,-0.7322445458,-5.4765758396\H,23.1568077161,0.1594234132,-5.6360198492\H,23.644225534,-1.4337197179,-6.3063331019\H,24.8191934087,-0.4698182499,-5.3777208333\H,25.0474040358,-3.022865005,-1.3847186971\H,23.7883442429,-4.1482883793,-0.8354195178\H,24.771949846,-4.5295597542,-2.2758073903\H,17.6900400764,-2.5424661298,-1.7404363291\H,16.3540130697,-3.5780590032,-2.2564373475\\Version=EM64L-G03RevE.01\State=1-A\HF=-2557.8786377\RMSD=7.482e-09\RMSF=4.730e-06\Thermal=0.\Di pole=0.8884561,-0.5211848,0.674777\PG=C01 [X(C20H33N1O7S3)]\@

n.S=CSMMMSM

1\1\GINC-X148\FOpt\RB3LYP\Gen\C17H26O8S3\CYL509\21-Apr-2009\0\#\B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134217280\n.S=CSMMMSM.a2.freq\0,1\C,5.0221552241,-4.4606177327,10.9430271674\C,5.3914894825,-5.7251379434,10.1405017718\C,5.4961439111,-5.4273638061,8.6498863856\O,5.3350380133,-6.5567115045,7.917437726\C,5.5128451381,-6.3976967827,6.4993345314\O,5.7228912049,-4.3447773405,8.1569249233\H,4.6144280428,-6.4881469034,10.2701377197\H,5.607211828,-3.6125122515,10.5706634471\H,5.3188382745,-4.6234534231,11.9859665468\H,5.3692849075,-7.392160284,6.0752830484\H,4.7744889741,-5.7002500841,6.0964089013\H,6.5162000752,-6.0213819591,6.2847972419\C,7.1913060753,-9.4471148999,12.4037974413\S,8.2280354558,-10.4717965415,13.4184283947\S,5.5478511387,-9.3326515819,12.4676518171\S,8.2705189495,-8.5691327045,11.3012815713\C,7.0590511033,-11.1764755182,14.6757696117\C,7.0988722738,-7.705337245,10.1463113078\C,6.7238289897,-6.3162800313,10.6846950669\C,6.5686922039,-12.5659532581,14.2779106908\H,6.2275674291,-8.3598869811,10.0669562236\C,7.8321660482,-7.6762967051,8.8065174581\O,8.4721936073,-6.7343721806,8.3921326216\O,7.7092865163,-8.8511144318,8.1648264649\C,8.4619174358,-8.9748973132,6.9449880363\H,8.2801210653,-9.99071299

99,6.5941956286\H,9.5263769379,-8.8170843104,7.1361678798\H,8.119916123,-8.2456972657,6.2063800252\H,6.2370638459,-10.4599614251,14.7422176088\C,7.8307862928,-11.1933174933,15.9923158512\O,8.5087658275,-12.1198316335,16.3784537368\O,7.6630799483,-10.0408771275,16.6657486251\C,8.3919466819,-9.937022773,17.9029151618\H,8.1416016376,-8.9557673176,18.3057538731\H,9.4664175838,-10.0167329955,17.7190507193\H,8.0870312477,-10.727997539,18.5927327194\H,5.8648927465,-12.9372429908,15.0321630612\H,6.0528983669,-12.5234213621,13.3154908094\H,7.4021359845,-13.2695340315,14.2156968575\H,6.6058937477,-6.4017149257,11.7680704465\H,7.5507671755,-5.6240515194,10.49394166\C,3.518842321,-4.0791711201,10.9719706956\H,2.9445012726,-4.9859234899,11.2000701263\C,3.2539744929,-3.0174891067,12.0481528187\H,3.8033548881,-2.0981831401,11.825539545\H,3.5657590659,-3.3855458576,13.0315988746\H,2.1905074844,-2.762700613,12.0989326012\C,3.0372935682,-3.5657468165,9.621325361\O,2.9862580427,-2.4025906926,9.2900723291\O,2.6556955842,-4.5864448739,8.8129997606\C,2.2561324668,-4.1926001926,7.4892296378\H,1.4113919879,-3.5004643559,7.5338397525\H,1.9688192427,-5.1155933253,6.9837904966\H,3.0896630669,-3.7082292981,6.9741752204\Version=EM64L-G03RevE.01\State=1-A\HF=-2459.8556265\RMSD=7.562e-09\RMSF=5.864e-07\Thermal=0.\Dipole=-0.2949566,-1.2537206,0.0005613\PG=C01 [X(C17H26O8S3)]\@

r.I1

1\1\GINC-X45\FOpt\UB3LYP\Gen\C8H7O1S1(2)\CYL509\01-Mar-2009\0\#\B3LYP/gen 6D INT(grid=ultrafine) OPT maxdisk=1342177280\r.I1_a10.freq\0,2\H,-0.0436479942,0.0377547646,0.0958275761\C,-0.0122576216,-0.0051149976,1.1877056095\S,1.7011920518,-0.0284951275,1.8090667375\H,-0.4560083169,0.908985212,1.5896819073\H,-0.583395992,-0.863832636,1.5502392027\C,2.3789089756,-1.5228616811,1.1337783228\C,3.7231752299,-1.7993400951,1.4608909227\C,4.3400734306,-2.9421319235,0.9810787597\C,3.6301564457,-3.8408508836,0.160522051\C,2.2972028917,-3.5648830825,-0.1627000413\C,1.6708984678,-2.4172460328,0.3166485904\H,0.6373397497,-2.2276248806,0.0509583084\H,4.2747100998,-1.1086596898,2.093636963\H,5.3745480238,-3.1597659498,1.2298214217\H,1.7535963507,-4.2607129306,-0.7957589582\C,4.2666009289,-5.0642302177,-0.362097994\O,5.3856200543,-5.450520929,-0.1866608366\Version=EM64L-G03RevE.01\State=2-A\HF=-782.423046\S2=0.752902\S2-1=0.\S2A=0.750006\RMSD=9.035e-09\RMSF=4.276e-06\Thermal=0.\Dipole=-1.3903039,1.0610411,0.1422039\PG=C01 [X(C8H7O1S1)]\@

r.I1M

1\1\GINC-X10\FOpt\UB3LYP\Gen\C12H13O3S1(2)\CYL509\04-Mar-2009\0\#\B3LYP/gen 6D INT(grid=ultrafine) OPT maxdisk=1342177280\r.I1M.freq\0,2\H,3.022412275,0.3397901603,3.3582948115\C,2.8231467678,1.0356720387,2.5390981247\S,1.6694967785,0.3242465894,1.3201221447\H,2.3183451411,1.9181182335,2.9398947432\H,3.7608094679,1.3466915555,2.0710500557\C,2.5332512927,-1.0955779934,0.6961395999\C,3.808179181,-1.4988634535,1.1156747359\C,4.4090104891,-2.6279396255,0.5607145618\C,3.7478436739,-3.3830677689,-0.4190427996\C,2.4643825244,-2.9751943668,-0.8313213715\C,1.8657545299,-1.8520711947,-0.288091571\H,0.8758281132,-1.5503065404,-0.6202021574\H,4.3457846264,-0.9419022165,1.8745778684\H,5.3915877479,-2.9185609133,0.9193054082\H,1.9548017318,-3.5632205909,-1.587613689\C,4.3291402601,-4.5957394634,-1.0539538139\O,3.700376568,-5.2646979483,-1.8580857934\C,5.7662534295,-5.8835971987,0.5467895328\C,5.7700140158,-5.0393219359,-0.6753147801\H,6.4339938522,-4.1827791075,-0.5369926523\H,6.1111549129,-5.6272143567,-1.5356569463\C,6.4120191109,-5.4563279551,1.7722892467\O,6.3272077318,-6.4031839346,2.7416985534\C,6.9449694571,-6.0587184545,3.9887592643\H,8.0135881765,-5.8696784988,3.8520382967\H,6.7887525457,-6.9190510042,4.6403242726\H,6.4811675605,-5.1648388229,4.4158880432\O,6.9740637997,-4.3776813339,1.9373027131\H,5.2568552383,-6.8419138992,0.5380145976\Version=EM64L-G03RevE.01\State=2-A\HF=-1088.9307561\S2=0.756498\S2-1=0.\S2A=0.75003\RMSD=9.306e-09\RMSF=2.012e-0

6\Thermal=0.\Dipole=0.4307443,0.4746101,1.2070369\PG=C01 [X(C12H13O3S1)]\@

r.I1MM

1\1\GINC-X2\FOpt\UB3LYP\Gen\C16H19O5S1(2)\CYL509\07-Mar-2009\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT maxdisk=1342177280\r.I1MM confsearch\0,2\H,0.8641939734,2.0576317163,-0.2902608128\C,0.7147854565,1.7228203249,0.7391739925\S,2.2480247698,0.8492975382,1.1958996603\C,1.9596669175,0.3321136864,2.8700675015\C,3.0044377625,-0.3752630175,3.4967401703\C,2.8672481773,-0.8176085513,4.8016642038\C,1.6876515911,-0.5746770466,5.5285941705\C,0.6525418561,0.1300133295,4.8997985696\C,0.7812373921,0.5808525278,3.5872836181\C,1.6016618015,-1.0761795216,6.9298801449\O,2.5406884337,-1.6716227302,7.4434680274\C,0.3180352324,-0.8385884709,7.7221605399\C,0.3619176357,-1.4763462645,9.1153884958\C,1.4532359931,-0.8135553366,9.9466722256\O,2.062798644,-1.6897077677,10.7711530981\C,3.1105900741,-1.1377268196,11.5873839894\C,-1.0120251805,-1.3093681025,9.8248897392\C,-1.1451532641,-2.0694019793,11.0974341441\C,-2.3596182441,-2.8026641087,11.3977883556\O,-3.3334565743,-2.8883995763,10.6593674525\O,-2.2974566633,-3.3999514413,12.6193875981\C,-3.4619752284,-4.148604808,12.9883246837\O,1.7059034116,0.3730695758,9.9210397818\H,-0.3404433706,-2.0848455799,11.8247571435\H,-3.2480386634,-4.5563737914,13.9770656076\H,-3.6471438887,-4.9553986144,12.2730351742\H,-4.343888224,-3.5021482884,13.0231131913\H,-1.8193445624,-1.6167145476,9.1516163389\H,-1.1604193538,-0.232692823,10.0172211182\H,0.5980055435,-2.5398780481,9.0269999498\H,0.1576629495,0.2428428324,7.818432044\H,-0.5353356458,-1.2365289978,7.1580615225\H,3.4794121781,-1.9684535621,12.1895068115\H,3.9075239661,-0.7367003679,10.9562199292\H,2.7237346794,-0.3388751813,12.225564897\H,-0.1525335305,1.0580537428,0.7716369367\H,0.5456294576,2.5969130093,1.3736309341\H,-0.040681785,1.1239724552,3.1349523684\H,3.9234242892,-0.572784884,2.9511042008\H,3.6693125418,-1.3611762737,5.2901816982\H,-0.270924072,0.3410114181,5.4302913797\Version=EM64L-G03RevE.01\State=2-A\HF=-1395.4298804\S2=0.756549\S2-1=0.\S2A=0.75028\RMSD=7.819e-09\RMSF=2.080e-06\Thermal=0.\Dipole=-0.5431594,0.3049775,-0.3867539\PG=C01 [X(C16H19O5S1)]\@

r.I2

1\1\GINC-X42\FOpt\UB3LYP\Gen\C7H14N1O1(2)\CYL509\27-Feb-2009\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT maxdisk=1342177280\r.I2.freq\0,2\C,-2.317797079,2.1741351076,-2.346334693\C,-2.6537883933,1.7090081835,-0.9563923584\H,-2.7078030295,0.6164562503,-0.9363574598\H,-3.6217523736,2.0806697082,-0.5949874478\H,-1.8990843586,2.0080925923,-0.2043325034\C,-1.5305601759,1.2464785576,-3.2299750202\H,-1.7952261267,1.3282062621,-4.2925160337\H,-1.7192500728,0.2094988506,-2.9366053958\H,-0.4376124716,1.4064609102,-3.1628374911\N,-2.1481155917,3.564371251,-2.545304862\C,-1.4604822824,5.4856165718,-3.9157605706\C,-2.4742978028,5.9032100013,-1.8629456991\O,-2.3358905134,6.3471874122,-3.2041332212\C,-3.0139455028,4.4760678353,-1.7919678846\C,-1.963871666,4.0435356302,-3.9181619958\H,-0.4513701727,5.5215551926,-3.4719068177\H,-1.5014515826,5.9540710379,-1.3456615286\H,-4.0469861662,4.4579901255,-2.1854946728\H,-2.9100806641,3.989705827,-4.4875243441\H,-1.4075686631,5.8700783699,-4.9390690346\H,-3.1677453114,6.5951304744,-1.3749393067\H,-3.0489537419,4.1689875149,-0.7442808801\H,-1.228474258,3.4191103338,-4.4304817791\Version=EM64L-G03RevE.01\State=2-A\HF=-405.0798005\S2=0.753382\S2-1=0.\S2A=0.750009\RMSD=8.517e-09\RMSF=7.661e-06\Thermal=0.\Dipole=0.1190682,-0.2702564,0.1138347\PG=C01 [X(C7H14N1O1)]\@

r.I2M

1\1\GINC-X6\FOpt\UB3LYP\Gen\C11H20N1O3(2)\CYL509\04-Mar-2009\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT maxdisk=1342177280\r.I2M.freq\0,2\C,-0.0447361445,0.3805999484,1.0654958672\C,-0.7220362713,-0.5338250643,

1.9649094113\O,-1.3365450003,-1.5372699356,1.6251940925\O,-0.594081648
4,-0.1463180922,3.265573006\C,-1.2367635309,-1.0017134342,4.218080942\
H,-2.3125258927,-1.0566730664,4.0268602714\H,-1.0447094523,-0.55276670
35,5.1934977848\H,-0.8219398025,-2.0131623702,4.1738086627\C,-0.088057
8486,0.1946880448,-0.4073699306\H,-0.4117178255,1.1435617386,-0.856094
1924\H,-0.8325060857,-0.5659916579,-0.6567644845\C,1.2690446761,-0.230
9436507,-1.0836793377\C,2.3750751224,0.8065113562,-0.7895643694\H,2.62
5307008,0.8177923889,0.2768592824\H,2.0743505984,1.8214938992,-1.07116
88824\H,3.2911685552,0.5624679009,-1.3397686249\C,1.6795374286,-1.5876
404716,-0.4838967545\H,0.959865111,-2.3694886891,-0.7477161165\H,1.704
3596525,-1.5122165156,0.6070799337\H,2.677280516,-1.8979672159,-0.8092
457219\N,0.9843371615,-0.3801412923,-2.5395429403\C,0.1904144682,0.564
1351399,-4.6590187513\C,1.3344234781,-1.4630388232,-4.7098376066\O,1.0
769578984,-0.2539265465,-5.4072508801\C,1.9115266883,-1.211169923,-3.3
157189434\C,0.7554200843,0.8703456893,-3.2727215593\H,-0.7891712973,0.
0690753657,-4.5543636706\H,0.4057269587,-2.0495916143,-4.6133745204\H,
2.9099131165,-0.7441723291,-3.4232874856\H,1.6837961918,1.4573175048,-
3.4001070459\H,0.0608425649,1.4874361276,-5.2325408498\H,2.0466799776,
-2.0277885767,-5.3196946337\H,2.0455942092,-2.1801408135,-2.8307710282
\H,0.0381579497,1.4991440291,-2.7368985638\H,0.4880123846,1.2167216527
\,1.5084436397\Version=EM64L-G03RevE.01\State=2-A\HF=-711.5715084\S2=0
.756647\S2-1=0.\S2A=0.750028\RMSD=3.801e-09\RMSF=9.058e-06\Thermal=0.\
Dipole=0.4169671,0.4285508,0.6514482\PG=C01 [X(C11H20N1O3)]\@

r.I2MM

1\1\GINC-X1\FOpt\UB3LYP\Gen\C15H26N1O5(2)\CYL509\06-Mar-2009\0\#B3LYP
/gen 6D INT(grid=ultrafine) OPT maxdisk=1342177280\r.I2MM.a2.freq\0,
2\O,0.1512937798,-0.2207589068,0.0424830989\C,0.0658810804,-0.05743436
76,1.4494862012\C,1.4446409379,0.0671571156,2.1013747376\N,2.162642533
3,1.2050957719,1.5177074351\C,2.2680195419,0.9807793542,0.0698464188\C
,0.8715109824,0.8581484139,-0.5365326064\C,3.4313244673,1.628928223,2.
1923359595\C,3.2384771651,1.5943037774,3.7205748286\C,3.6612603642,3.1
124907448,1.7726913911\C,4.9947885296,3.7682955825,2.1858814378\C,6.12
02809676,3.3926694887,1.2328569658\O,7.2677669139,3.1239482126,1.89562
25442\C,8.4019592454,2.8139939327,1.0670660207\O,6.0309818102,3.375074
3202,0.0223665\C,4.6271414397,0.7212045804,1.8223088908\H,8.2043354193
,1.9222265753,0.4665989269\H,9.2278981629,2.6378997011,1.7565591984\H,
8.6289254243,3.6486805472,0.3986654947\H,3.5853624203,3.2155786452,0.6
869545556\H,2.8339444629,3.6910990414,2.1991882343\H,5.5148475545,0.97
91531222,2.4103853459\H,4.8928569226,0.8015295264,0.7640028536\H,4.390
7206732,-0.3278466532,2.0349106243\H,2.3164309626,2.1103891352,4.01047
5514\H,4.0734853011,2.0962412403,4.2178939016\H,3.2053189744,0.5724451
76,4.1112708363\H,0.3234547375,1.803865495,-0.3911231177\H,-0.52654072
1,0.8408598651,1.6914849374\H,1.9867388805,-0.8898800236,1.9705072083\
H,2.8278781084,0.0576179019,-0.1685312687\H,0.9352973736,0.6475594254,
-1.6088220693\H,-0.4583284714,-0.9388538876,1.8327217459\H,1.293522732
6,0.2219484458,3.1717150051\H,2.7897850901,1.8130688813,-0.4103123358\
H,5.2899882726,3.4926572411,3.2008867249\C,4.8417038135,5.3296727804,2
.1648012885\H,4.5387212568,5.6334330075,1.1568652124\H,4.0316962369,5.
5701575576,2.8625852554\C,6.0724925166,6.0594113366,2.5764073865\H,6.7
68830512,6.4527993774,1.8426979083\C,6.4056937438,6.1911002168,3.98217
19406\O,5.7319837522,5.7444351061,4.902892236\O,7.566499495,6.87404930
71,4.1700989563\C,7.9592983526,7.0384435792,5.5386470465\H,7.194728928
3,7.5850634896,6.0983269673\H,8.8909920909,7.6047593394,5.5110074273\H
,8.1153653139,6.0665033246,6.0158677251\Version=EM64L-G03RevE.01\Stat
e=2-A\HF=-1018.0680977\S2=0.756366\S2-1=0.\S2A=0.750027\RMSD=5.320e-09
\RMSF=1.899e-06\Thermal=0.\Dipole=1.1376307,0.3854934,0.4597942\PG=C01
[X(C15H26N1O5)]\@

r.MMM

1\1\GINC-AC52\FOpt\UB3LYP\6-31G(d)\C12H19O6(2)\CYL509\22-Aug-2007\0\#\#
B3LYP/6-31G* OPT MAXDISK=402653184 FREQ=NORAMAN\sample\0,2\H,-4.423
810185,-2.5955407348,-2.8988437604\C,-4.2536649881,-2.7893176254,-1.83
57418237\O,-2.852415586,-2.9040705929,-1.5580575528\H,-4.6959436256,-1
.9755224909,-1.2538121517\H,-4.6895596627,-3.7464035564,-1.5468315476\
C,-2.1140567825,-1.8030460561,-1.8548570916\C,-0.7140979058,-1.9832946
273,-1.5187060507\O,-2.5920651869,-0.7879885091,-2.3492155006\C,0.2718
898725,-0.8907156077,-1.7421863699\H,-0.4198311588,-2.9188632807,-1.05
41907551\C,0.5129148334,0.034829142,-0.4959789435\H,1.2449841119,-1.31
81119485,-2.0134713448\H,-0.0715838784,-0.2578827387,-2.5662167414\C,1
.0629120595,-0.7392861829,0.7100426445\H,1.2387649677,0.7874017687,-0.
8192505043\C,-0.7949241514,0.7403372095,-0.1627552281\C,1.5235688279,0
.1441553014,1.8794974199\H,0.2858827089,-1.4152056699,1.0815246773\H,1
.9104170965,-1.3494694828,0.3769265251\C,2.7300147536,0.990164144,1.49
35619208\C,1.877804547,-0.7040913948,3.1200961481\H,0.7160597223,0.828
4246397,2.1643019247\O,2.8980346624,2.0199235858,2.3540795385\O,3.4773
322867,0.7781274587,0.5602923435\C,4.0409213817,2.8546389669,2.1051193
099\H,3.9734745543,3.3123782151,1.1145549269\H,4.0200976069,3.61884496
64,2.8826670851\H,4.9640867942,2.2717333386,2.1635026152\O,-1.00075538
52,1.7912745208,-0.9791465289\O,-1.5775526248,0.3879633392,0.696684840
9\C,-2.2986027052,2.4047597534,-0.8818662107\H,-2.2755187429,3.2456409
862,-1.5757070469\H,-2.4854008957,2.7507017113,0.1379477842\H,-3.06660
01267,1.6849174916,-1.1739417099\H,2.6850437459,-1.410392239,2.8929491
132\H,1.0028420065,-1.2787113124,3.4410043063\H,2.1978911756,-0.070576
2208,3.9524351283\Version=IA64L-G03RevC.02\State=2-A\HF=-920.0484442\
S2=0.756383\S2-1=0.\S2A=0.750027\RMSD=6.713e-09\RMSF=2.457e-06\Dipole=
0.1290022,0.0661614,0.3046913\PG=C01 [X(C12H19O6)]\@

r.SM3

1\1\GINC-X5\FOpt\UB3LYP\Gen\C13H21O6S3(2)\CYL509\02-Mar-2009\0\#\#B3LYP
/gen 6D INT(grid=ultrafine) OPT maxdisk=1342177280\r.Sma3_c34.freq\0
2\C,-0.030388243,-0.3065152873,-0.0107741714\S,-0.1412749746,-0.15985
58201,1.7429635194\S,1.5676873846,-0.2053549448,-0.7488996771\S,-1.418
0655388,0.2033732994,-0.9717292846\C,0.8473194177,-1.6014297183,2.3780
62364\C,-2.7895869338,-0.9215483464,-0.4126517725\C,1.4625208938,-1.35
43030378,-2.2076938052\C,-4.119716595,-0.2714727966,-0.8159333383\C,1.
2193394185,-1.3055758073,3.8370557635\H,-2.7128149466,-1.0074497008,0.
6727919455\C,-2.6489655634,-2.3307115566,-0.9739957581\O,-2.522348032,
-3.319375704,-0.2817417114\O,-2.7322671679,-2.3547279421,-2.31291571\C
, -2.5871685567,-3.6550184069,-2.9228426952\H,-2.7346317841,-3.48689977
12,-3.9902483446\H,-3.3431544412,-4.3420689723,-2.5341080744\H,-1.5875
956484,-4.0422794246,-2.7216558502\H,1.7416803825,-1.6768240286,1.7568
844328\C,0.1032043946,-2.9229297614,2.2349574697\O,0.5111235377,-3.854
4927024,1.572786441\O,-1.0243323828,-2.9522467546,2.9616304673\C,-1.79
84362117,-4.1664836277,2.8612879928\H,-2.6336164705,-4.0293928476,3.54
90400735\H,-1.1933247332,-5.0269053941,3.158344133\H,-2.1510074115,-4.
2901606085,1.8366527607\H,0.4890427082,-1.1931952505,-2.6744598251\C,2
.5980603293,-0.9881275738,-3.1726280403\C,1.5128616946,-2.8201612518,-
1.7962851053\O,0.6187843204,-3.6104616837,-2.0171159715\O,2.6759595994
, -3.143523078,-1.2107176926\C,2.7928423586,-4.5139803571,-0.77278642\H
, 2.0494732514,-4.7146907518,-0.0003928895\H,3.804407446,-4.6003505799,
-0.3745100874\H,2.6529349573,-5.1942799129,-1.6168251603\H,1.802930764
, -2.1376961026,4.2467016682\H,1.8241297729,-0.3963894361,3.8997926606\
H,0.3262745044,-1.1806035619,4.4558899094\H,-4.9538415786,-0.909856405
9,-0.503670392\H,-4.2307106348,0.7026845253,-0.3311297736\H,-4.1824628
807,-0.1373244403,-1.8995441576\H,2.569573369,-1.6488382591,-4.0464046
509\H,2.4879712552,0.0441134639,-3.5171290295\H,3.5753956835,-1.099915
3778,-2.6946733781\Version=EM64L-G03RevE.01\State=2-A\HF=-2153.924285
3\S2=0.755525\S2-1=0.\S2A=0.750023\RMSD=5.154e-09\RMSF=4.260e-05\Therm
al=0.\Dipole=-0.0430929,-0.3426075,-0.0253742\PG=C01 [X(C13H21O6S3)]\@

@

n.SM2

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1\1\GINC-X146\FOpt\RB3LYP\Gen\C9H14O4S3\CYL509\05-Mar-2009\0\#\B3LYP/gen
6D INT(grid=ultrafine) OPT maxdisk=1342177280\n.SM2 confsearch\0,
1\C,1.2235191852,1.1741272795,0.6100216186\S,1.2232507031,0.8073287795
,2.3485022765\S,2.4284361893,0.8512886649,-0.4666146844\S,-0.332615729
2,1.9579071573,0.2622966394\C,2.7636408283,-0.1989251095,2.5883433637\
C,-0.1666845201,2.5069023028,-1.5023306701\C,-0.7846010706,1.501190800
1,-2.4698901023\C,3.9335484551,0.6588991243,3.0625856175\H,0.906479437
9,2.6239710989,-1.670268624\C,-0.8473377425,3.87061081,-1.5769651043\O
,-2.0179873944,4.0405101398,-1.8379293562\O,0.0234168709,4.8609254849,
-1.3100645038\C,-0.5332879868,6.1882695611,-1.3066466377\H,0.299696674
1,6.8517990189,-1.074831349\H,-1.3157395571,6.2707228498,-0.5479109917
\H,-0.957274627,6.4267499637,-2.2853842998\H,2.9649434315,-0.657579629
9,1.6174217173\C,2.3969481893,-1.2818695406,3.5989441125\O,2.516000466
5,-1.1697998264,4.7992188193\O,1.9190239225,-2.3775773665,2.9815424217
\C,1.4967437322,-3.4425063823,3.8529726945\H,1.1432884259,-4.234654539
4,3.1930913151\H,0.6935303474,-3.1001762046,4.5105178667\H,2.334107133
9,-3.7914529835,4.462581915\H,4.8279659744,0.0340024941,3.1703044706\H
,4.1463154204,1.4438128478,2.3327222309\H,3.7162429293,1.1108945314,4.
0331939144\H,-0.6464930209,1.8494207307,-3.5002982065\H,-0.2973601595,
0.5286787198,-2.365611172\H,-1.8566509639,1.3947147048,-2.2882963575\
Version=EM64L-G03RevE.01\State=1-A\HF=-1846.8607543\RMSD=8.150e-09\RMS
F=1.460e-06\Thermal=0.\Dipole=0.2990357,-0.0802282,-0.2670136\PG=C01 [
X(C9H14O4S3)]\@
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r.M

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1\1\GINC-SC160\FOpt\UB3LYP\6-31G(d)\C4H7O2(2)\MLC501\30-Jul-2003\0\#\
B3LYP/6-31G* OPT=TIGHT FREQ MAXDISK=39321600 GEOM=CHECK GUESS=READ\MA
_rad-csc-6dub3 (EA conf)\0,2\C,2.4427069032,-0.6700725424,0.\C,0.9884
454995,-0.9680099437,0.\C,0.0000531191,0.0925714969,0.\O,0.2492141423,
1.2915528696,0.\O,-1.2690884584,-0.4038514401,0.\C,-2.3055213085,0.584
7337423,0.\H,-3.2434106254,0.0277541879,0.\H,2.6133119038,0.4089560571
,0.\H,0.6334677625,-1.9941959598,0.\H,2.9379202621,-1.1090091687,0.878
9917495\H,2.9379202621,-1.1090091687,-0.8789917495\H,-2.2371601584,1.2
192780488,0.8886413064\H,-2.2371601584,1.2192780488,-0.8886413064\Ver
sion=DEC-AXP-OSF/1-G03RevB.03\State=2-A\HF=-307.0484404\S2=0.756686\S
2-1=0.\S2A=0.750029\RMSD=9.256e-09\RMSF=1.294e-06\Dipole=-0.0936169,-0
.6405142,0.\PG=CS [SG(C4H3O2),X(H4)]\@
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n.SiPr2

```
1\1\GINC-X96\FOpt\RB3LYP\Gen\C7H14S3\CYL509\16-Mar-2009\0\#\B3LYP/gen
6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1342177280
\n.SiPr2.freq\0,1\C,1.2236045175,1.1741706196,0.6099963821\S,1.10314
55107,0.5625458105,2.2696458614\S,2.4139556838,0.8197659669,-0.4814860
221\S,-0.1696413408,2.2362718826,0.3382034823\C,2.7116797598,-0.311158
0286,2.5728326753\C,-0.1291415756,2.6193418645,-1.4768258526\C,-0.7192
527946,1.4767102133,-2.3041770353\C,3.8288613945,0.6747004991,2.916900
9766\H,0.9292491206,2.7482256816,-1.7209019158\H,2.9428444538,-0.82373
34475,1.6346415929\H,4.767163601,0.125823527,3.0679250878\H,3.98579974
25,1.3941835753,2.1091499743\H,3.6017144711,1.223013707,3.8376997179\H
,-0.6588611968,1.7284655853,-3.3706948839\H,-0.1677555826,0.5463478079
,-2.1459901659\H,-1.7720273305,1.3093175871,-2.0516684345\C,-0.8808951
87,3.9406468903,-1.6693809361\H,-0.4188216983,4.7563846225,-1.10504900
08\H,-1.9296778838,3.8581994663,-1.3610189019\H,-0.8687272642,4.208682
3074,-2.732289771\C,2.4595632875,-1.333741001,3.6858417059\H,3.3876008
153,-1.8816986013,3.8864833238\H,1.6883191829,-2.057407356,3.404944463
1\H,2.1536195482,-0.8481137289,4.6198626681\Version=EM64L-G03RevE.01\
State=1-A\HF=-1469.7552639\RMSD=2.948e-09\RMSF=4.414e-06\Thermal=0.\Di
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pole=-0.071733,0.0241897,0.0638556\PG=C01 [X(C7H14S3)]\@

r.SI1SiPr2

1\1\GINC-X123\FOpt\UB3LYP\Gen\C15H21O1S4(2)\CYL509\17-Mar-2009\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT maxdisk=1342177280\r.SI1SiPr2 confs earch\0,2\H,1.2972762942,1.3541341687,0.146576255\C,1.124558698,1.2615334596,1.2216152275\S,2.1311201998,-0.1609572639,1.7564668092\C,1.8108065061,-0.2766692312,3.4985190096\C,2.4653855426,-1.3150847832,4.1891485577\C,2.2762026158,-1.4802749429,5.5510273592\C,1.4232003489,-0.6215996766,6.2690699416\C,0.7791462173,0.4148881317,5.5803863415\C,0.9678149516,0.5880895043,4.211318881\C,1.2631575497,-0.8735254717,7.7240272174\O,1.9745842349,-1.6314732422,8.3506151107\S,-0.1389155052,0.0194669859,8.5162503811\C,0.1483068319,-0.2737918349,10.2312433538\S,-1.0931092648,-1.0449292685,11.2096146328\C,-1.4699751042,-2.6375002744,10.3178740319\C,-0.2834343357,-3.6002689127,10.3382131185\S,1.3737456727,0.7042934334,11.0197494647\C,2.185473775,-0.4521584833,12.2438620954\C,2.7086877513,0.3984333841,13.4039766108\C,3.2836647772,-1.276501463,11.5715691014\C,-2.7222875865,-3.2216633164,10.9782812584\H,1.3842795381,-1.1063593243,12.599810141\H,2.7816669096,-2.2774117561,6.0858792379\H,0.1376696516,1.1105177697,6.1121945589\H,0.4589371881,1.4046511538,3.712224381\H,3.1240888779,-1.9899682089,3.6490540793\H,0.0591887946,1.0879466923,1.3945699613\H,1.4421546509,2.1860402254,1.710992177\H,3.693870707,-2.0010980683,12.2880529269\H,2.9017299037,-1.8171901649,10.7027427061\H,4.1038910739,-0.6323867796,11.2341591723\H,-1.7011510287,-2.3551243238,9.2856284111\H,-2.5391939395,-3.4667677983,12.0310956914\H,-3.0075807524,-4.1476069032,10.4654366212\H,-3.5687068894,-2.5292037,10.9285405179\H,-0.0247561147,-3.8819604748,11.3654489242\H,0.595317236,-3.1552965336,9.8639827065\H,-0.5420908876,-4.5156426692,9.7894963551\H,3.2073414047,-0.247202041,14.1369946155\H,1.8996935422,0.9341757167,13.909754024\H,3.4448104362,1.1345328147,13.058727918\Version=EM64L-G03RevE.01\State=2-A\HF=-2252.2028588\S2=0.755684\S2-1=0.\S2A=0.750024\RMSD=6.961e-09\RMSF=1.373e-06\Thermal=0.\Dipole=-0.2781319,-0.1046071,-0.9884917\PG=C01 [X(C15H21O1S4)]\@

r.SMI1SiPr2

1\1\GINC-X129\FOpt\UB3LYP\Gen\C19H27O3S4(2)\CYL509\18-Mar-2009\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=norman maxdisk=1342177280\r.SMI1SiPr2.freq\0,2\S,0.14257864,0.3909124857,8.7240410239\C,0.4346288741,-0.3561902483,10.303554859\S,-1.0012277423,-0.7282842301,11.2674278714\C,-1.9413561693,-1.9552497497,10.2240661842\C,-1.1872238696,-3.2740686776,10.0669413431\S,1.9297664768,0.0222736881,11.1675791551\C,2.3208895496,-1.5616897606,12.0689029507\C,3.3135026164,-1.2138420081,13.1816933361\C,2.8564144834,-2.6365544211,11.1234327271\C,-3.3098410774,-2.1357406048,10.8868366404\H,1.3757618061,-1.8917542386,12.5111887338\H,3.0338167264,-3.5699725393,11.6738658875\H,2.1433509907,-2.849678736,10.320971308\H,3.8042342688,-2.324594495,10.6695058873\H,-2.0701235458,-1.4846842771,9.2447347491\H,-3.2116075396,-2.5563073129,11.8947055083\H,-3.9185275288,-2.8283436496,10.2935751213\H,-3.8492666558,-1.1863961268,10.9622831562\H,-1.0377050577,-3.7610447523,11.0373235776\H,-0.2062895201,-3.1154452089,9.6082147394\H,-1.7567393621,-3.958496943,9.4244110168\H,3.5652586096,-2.117899297,13.7489047003\H,2.8969891571,-0.4778645387,13.8761053019\H,4.2464496925,-0.8087207101,12.7715292134\C,1.6441884692,-0.1163519199,7.7632962916\C,1.3000410113,-1.0550613492,6.6038255289\H,2.2673566531,-0.6561770246,8.4849518396\C,2.5009539677,1.0493351387,7.2650274704\O,3.1934565468,0.9727883943,6.2707916316\O,2.4724726638,2.1124904648,8.0783076111\C,3.3086493801,3.212670844,7.6828909692\H,3.1569795238,3.9786671347,8.4433078743\H,3.0101678515,3.5805303608,6.6980622991\H,4.356944695,2.9042897074,7.6476502154\H,2.2299124701,-1.3755609481,6.1188217962\H,0.8068067772,-1.9548028163,6.9905154949\H,0.4279181886,-4.9112906095,0.564165824\C,-0.663770727

8,-4.9677677509,0.5792278369\S,-1.4209736981,-3.3100556183,0.548638332
2\H,-1.0041923647,-5.4620650266,-0.333974967\H,-1.0007802608,-5.549094
8485,1.4416323178\C,-0.830959007,-2.5462284623,2.0392796273\C,0.008892
3394,-3.1690141514,2.9730276684\C,0.4161831003,-2.4817482832,4.1150381
351\C,0.0007162568,-1.1652956211,4.3550516198\C,-0.8412839971,-0.54817
49235,3.4121060474\C,-1.2519824115,-1.2226146352,2.2746948687\H,-1.901
9948125,-0.7290811428,1.5569747954\H,0.3521626513,-4.1859355961,2.8205
236232\H,1.0697362529,-2.9889472135,4.8181959042\H,-1.1611369477,0.471
8888483,3.5979121691\C,0.4068027204,-0.3885327454,5.5590040587\O,0.031
7518848,0.7656691456,5.7209881246\\Version=EM64L-G03RevE.01\State=2-A\
HF=-2558.6884337\S2=0.755351\S2-1=0.\S2A=0.750021\RMSD=8.768e-09\RMSF=
2.670e-06\Thermal=0.\Dipole=0.3626086,-2.1987753,-0.3078188\PG=C01 [X(
C19H27O3S4)]\@

r.SMMI1SiPr2

1\1\GINC-X133\FOpt\UB3LYP\Gen\C23H33O5S4(2)\CYL509\18-Mar-2009\0\#\B3L
YP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=134
2177280\r.SMMI1SiPr2.2.freq\0,2\H,6.8856982274,0.2597333309,8.457093
3623\C,7.2848222665,-0.5711878385,7.87020181\S,6.50094375,-0.432179193
1,6.2305215925\C,7.1917304918,-1.7874919434,5.3135274352\C,6.774581160
1,-1.9158636274,3.9742026437\C,7.2611010906,-2.943841642,3.1841429552\
C,8.1772694602,-3.8801212502,3.6964968743\C,8.5887248255,-3.7462616433
,5.0290556045\C,8.1055809603,-2.7148649465,5.8326610368\C,8.661344824,
-4.9658583709,2.795066394\O,8.2836115462,-5.0299650496,1.6322808412\C,
9.6236586346,-6.0129521973,3.3539060001\C,10.0647880352,-7.0305107421,
2.2953860556\C,10.9213913983,-6.3193903249,1.2543527819\O,10.840055387
5,-6.9268443759,0.0509162699\C,11.6597779567,-6.3471373357,-0.97871255
65\O,11.6114780339,-5.3474494989,1.4704438513\H,9.1815281503,-7.421580
9501,1.7806911584\H,10.504923144,-5.5074059208,3.7655962868\H,9.131937
8523,-6.527731525,4.1906633386\H,11.459198069,-6.9343589,-1.8755518587
\H,11.3877811144,-5.3005596489,-1.135600301\H,12.7147029201,-6.4083712
404,-0.6990846419\H,7.0223221259,-1.5103381666,8.364545934\H,8.3713238
77,-0.4683486468,7.8059564313\H,8.4488433865,-2.642470724,6.8584246125
\H,6.068268194,-1.2012072293,3.5598244649\H,6.9454189476,-3.0465238825
,2.1510729746\H,9.2993812051,-4.4461021057,5.4578062186\C,11.068892343
8,-9.4251459151,2.0611768808\C,10.8233992463,-8.2085830196,2.962653745
9\H,10.1874170417,-9.6879698221,1.4711870057\C,12.2581259714,-9.263212
3696,1.1233787879\O,13.2354986192,-8.5851740227,1.3621454931\O,12.1104
291346,-10.0126618349,0.0170320263\C,13.234742753,-10.0263389153,-0.87
74123063\H,12.9567143782,-10.7061293632,-1.6830052328\H,14.1291993452,
-10.3853562455,-0.3616678506\H,13.4275812644,-9.0244207942,-1.26961523
1\H,10.216827059,-8.5445361671,3.8104109076\H,11.7821663799,-7.8624362
92,3.3635544899\S,11.4684424759,-10.9481354417,3.0750265725\C,9.868236
5689,-11.6209111878,3.4178809244\S,9.6782497728,-12.4832246595,4.94889
81456\C,9.9990494861,-11.1858578185,6.24888296\C,8.8275473026,-10.2135
082306,6.3825680841\S,8.8687396487,-12.1285916963,2.0544096818\C,7.131
8807547,-11.7537089143,2.61938808\C,6.1852815,-12.5674223654,1.7325730
435\C,6.8335043096,-10.2554575154,2.5730654009\C,10.2970284933,-11.926
494246,7.5556781641\H,7.0713094087,-12.116563731,3.6501864662\H,5.8215
731106,-10.0609597466,2.9517829478\H,7.5388477531,-9.6906704987,3.1906
158926\H,6.8920997706,-9.8728865117,1.5478173313\H,10.894764165,-10.64
97214567,5.9204451795\H,9.4415609018,-12.5345586664,7.8734083193\H,10.
5029832376,-11.2012599056,8.3517790806\H,11.1666075913,-12.5831599656,
7.4567109471\H,7.9188767702,-10.7333611047,6.7066447397\H,8.6133935662
, -9.7146885857,5.4322105424\H,9.0627419279,-9.441373535,7.1269904535\H
,5.1476659761,-12.3837434766,2.0354796508\H,6.3815169566,-13.640903522
1,1.8129814522\H,6.2794199797,-12.2786218679,0.6789596533\\Version=EM6
4L-G03RevE.01\State=2-A\HF=-2865.1891415\S2=0.75546\S2-1=0.\S2A=0.7500
22\RMSD=8.384e-09\RMSF=1.269e-06\Thermal=0.\Dipole=-0.8305418,0.168312
8,1.293041\PG=C01 [X(C23H33O5S4)]\@

r.SI2SiPr2

```
1\1\GINC-X36\FOpt\UB3LYP\Gen\C14H28N1O1S3(2)\CYL509\17-Mar-2009\0\#\#B3
LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=13
42177280\r.SI2SiPr2.freq\0,2\C,-3.3951124584,5.9544049267,17.5167484
967\C,-4.222049862,5.9909809554,18.8087286518\H,-5.2733389829,6.156308
8757,18.5652249638\H,-3.9204747436,6.7939825397,19.4836855381\H,-4.122
0602925,5.0306169777,19.3308443646\C,-4.0437127392,4.9802031107,16.530
288182\H,-3.6074403245,5.0261748648,15.5308144537\H,-5.1069634234,5.20
73065312,16.4363915632\H,-3.9376752235,3.9584994571,16.9156228241\N,-2
.0162205981,5.6121582518,17.7834535903\C,0.1494399534,4.677100555,17.1
085094619\C,-0.0143253377,5.6772002211,19.2029930148\O,0.8313253853,5.
4449369007,18.0873475176\C,-1.2991140936,6.3991535394,18.7985817332\C,
-1.1315150667,5.3649722807,16.6363893229\H,-0.0976916836,3.6810114549,
17.5127927558\H,-0.2696977485,4.7215102374,19.6908824033\H,-1.04240087
47,7.404482171,18.4237986368\H,-0.872582902,6.3027269136,16.1176106264
\H,0.8421795678,4.553846151,16.2702738385\H,0.5577910788,6.2897256673,
19.9064739424\H,-1.921286848,6.5202818724,19.6867867321\H,-1.625923730
8,4.7082763907,15.9180190949\S,-3.4185808256,7.7704440327,16.729275518
3\C,-4.911817243,7.9916744604,15.8201279561\S,-4.8137902469,8.87678386
92,14.2828338094\C,-3.6854927209,7.8351888931,13.2331036562\C,-4.38422
24801,6.582552907,12.7044600204\S,-6.4150773325,8.1646895074,16.745279
6538\C,-7.7752939762,7.6998249013,15.5607602813\C,-9.0862721041,8.1819
485585,16.189833413\C,-7.7923444424,6.2026110477,15.2554172269\C,-3.16
40734639,8.7315812666,12.1059039852\H,-7.5832274045,8.2610251429,14.64
18248693\H,-8.5968062225,5.9740083513,14.5438955194\H,-6.847895947,5.8
771251143,14.8099626836\H,-7.9664152303,5.6165624905,16.1652538503\H,-
2.8554028243,7.5529836495,13.8884146295\H,-3.9836486145,9.0963477062,1
1.4750623438\H,-2.4813115952,8.1606423803,11.4652560509\H,-2.623173976
7,9.5976340438,12.4990272312\H,-5.2273589401,6.8461123794,12.055883945
\H,-4.7634834262,5.963969134,13.5231842656\H,-3.680194704,5.9766248433
,12.1183336836\H,-9.9233741853,7.9484419631,15.5212371064\H,-9.0769139
672,9.2625402379,16.3625191752\H,-9.2764581781,7.6830832736,17.1477284
172\Version=EM64L-G03RevE.01\State=2-A\HF=-1874.838502\S2=0.755451\S2
-1=0.\S2A=0.750022\RMSD=6.179e-09\RMSF=2.880e-06\Thermal=0.\Dipole=-0.
4461032,-1.1508914,-0.4256557\PG=C01 [X(C14H28N1O1S3)]\@
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r.SMI2SiPr2

```
1\1\GINC-X132\FOpt\UB3LYP\Gen\C18H34N1O3S3(2)\CYL509\18-Mar-2009\0\#\#B
3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1
342177280\r.SMI2SiPr2.freq\0,2\C,12.6894966514,1.2424501253,17.38775
10385\C,14.0829850872,1.3915852288,18.0379968974\H,12.7137928269,1.348
8412763,16.3029561616\C,12.0326146703,-0.0750388878,17.7701263135\O,11
.9152747781,-0.4869417608,18.9032025399\O,11.6175723812,-0.7588663067,
16.6790067087\C,10.9566496492,-2.0052937595,16.9582313185\H,10.7161917
55,-2.4333410398,15.9846277137\H,10.0469758414,-1.8278208258,17.537309
2326\H,11.6161343133,-2.6714028304,17.5202146884\H,14.3729353133,2.446
4183811,18.0130766044\H,13.9621975303,1.1198396293,19.0899576052\O,18.
7860127204,0.6453703274,19.9454333631\C,18.8333201182,1.2606186785,18.
6680174362\C,17.7775498572,0.6952869627,17.7153557998\N,16.4432800929,
0.8746992962,18.297605522\C,16.4191193513,0.1950466962,19.600235482\C,
17.4913313943,0.7877414992,20.5124611053\C,15.2700500013,0.5939349641,
17.4094549263\C,15.5380254888,1.1657271042,16.0044704213\C,14.97743090
77,-0.9181336533,17.2824246365\H,14.2083322692,-1.1082961024,16.526978
9767\H,14.6335463021,-1.3519211922,18.2261216324\H,15.8812349539,-1.45
420919,16.970338974\H,15.8715470968,2.2078484794,16.0603145037\H,14.62
36298209,1.1349731409,15.4048107866\H,16.2893125151,0.585781779,15.459
7785643\H,17.2704065579,1.8521658154,20.6960543594\H,18.6813575334,2.3
486263535,18.7651964543\H,18.0139341188,-0.367946181,17.5141649286\H,1
6.6086797822,-0.8900159204,19.5065940811\H,17.5132557451,0.2604360946,
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21.4713497153\H,19.8379556454,1.0790501627,18.2727216154\H,17.85673514
8,1.2399537685,16.7722147621\H,15.4438575396,0.3179563597,20.078781415
4\S,11.6882405371,2.6917882476,18.0440063687\C,10.3767342539,2.9552769
083,16.9109851585\S,10.2046056239,4.5937332643,16.2901049695\C,8.50575
9272,5.137341987,16.8536694913\C,8.4317811333,5.2454245964,18.37521886
96\S,9.1517398293,1.7152300743,16.6660266993\C,8.8651336272,1.71810713
82,14.8206778698\C,7.7125739026,0.7451203591,14.5575192906\C,10.132097
912,1.3575833067,14.0474508244\C,8.2129576077,6.4643848327,16.14922167
58\H,8.5522064904,2.733643757,14.5572347322\H,9.9213961757,1.352451027
2,12.9700349625\H,10.9255189888,2.0884480581,14.2307952265\H,10.501734
6429,0.3684724295,14.336683079\H,7.8040285584,4.3728663289,16.50477188
21\H,8.9327222875,7.2370789884,16.443500098\H,7.2127986704,6.816676727
9,16.428056156\H,8.2466418862,6.3619738555,15.05962107\H,9.1341392481,
5.9982560355,18.7497863842\H,8.6635298749,4.289627536,18.8547542277\H,
7.4183520526,5.5384774077,18.6795292491\H,7.4693984321,0.7430399057,13
.4885112126\H,6.8100708425,1.0248997996,15.1108694695\H,7.9848593922,-
0.2782720446,14.8406507489\Version=EM64L-G03RevE.01\State=2-A\HF=-218
1.3275969\S2=0.756115\S2-1=0.\S2A=0.750028\RMSD=6.144e-09\RMSF=9.876e-
07\Thermal=0.\Dipole=-1.0042698,-0.2327464,-1.5662527\PG=C01 [X(C18H34
N1O3S3)]\@

r.SMMI2SiPr2

1\1\GINC-X137\FOpt\UB3LYP\Gen\C22H40N1O5S3(2)\CYL509\18-Mar-2009\0\#B
3LYP/gen 6D INT(grid=ultrafine) OPT IOP(2/17=4) Freq=noraman maxdisk=1
342177280\@r.SMMI2SiPr2.2.freq\0,2\O,12.3500878895,-0.4620943857,-4.8
02534295\C,12.2260921948,-1.1456464986,-3.5656982394\C,12.7918803057,-
2.5661353487,-3.6306960023\N,14.2039685644,-2.5133599945,-4.0230048439
\C,14.2869335784,-1.8400884785,-5.3264823467\C,13.7092408892,-0.430732
9968,-5.216044282\C,14.9920443216,-3.7825333834,-3.9114125576\C,14.627
0032297,-4.499035236,-2.5967545733\C,16.4864042216,-3.3459571483,-3.81
64614117\C,17.5621643949,-4.4543066922,-3.8764377318\C,17.8121686079,-
4.8691744803,-5.3224263645\O,18.0173333747,-6.2029939703,-5.4303931668
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