

SUPPORTING INFORMATION

Polymerization of Vinyl Chloride at Ambient Temperature using Macromolecular Design via the Interchange of Xanthate: Kinetic and Computational Studies

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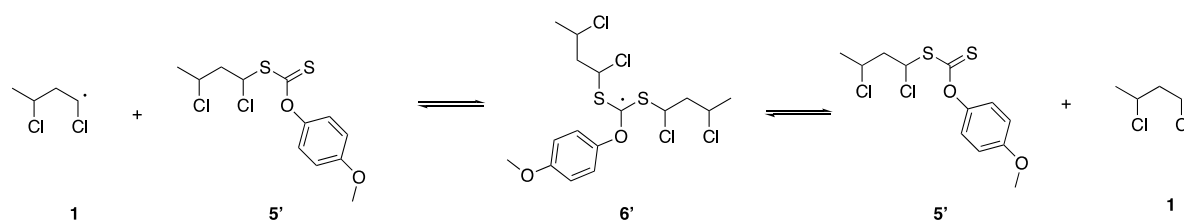
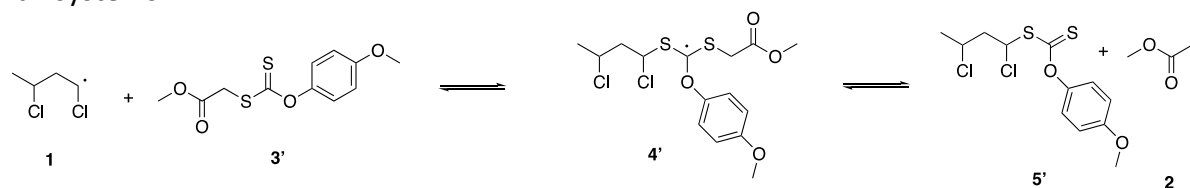
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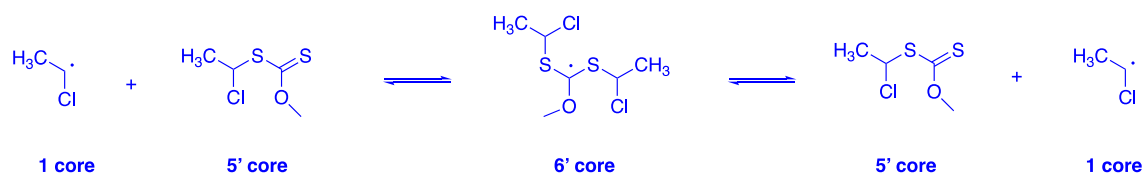
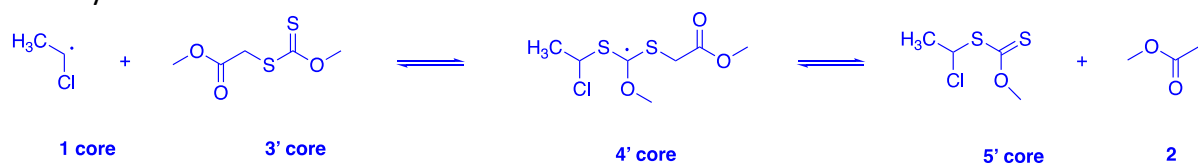
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Appendix S1. ONIOM Calculation Design

Full systems:



Core systems:



ONIOM Approximation:

Full_X @ G3(MP2)-RAD = Full_X @ ROMP2/6-311+G(3df,2p) + Core_X @ G3(MP2)-RAD - Core_X @ ROMP2/6-311+G(3df,2p)

Table S1. Thermodynamic parameters (in a.u.) for each species calculated at M062X/6-31G(d) level of theory in the gas phase at 42 °C.

T=315.15 K	E_{M06-2X}	$ZPVE_{M06-2X}$	TC_{M06-2X}	S_{M06-2X}^a	H_{M06-2X}	G_{M06-2X}
1	-1076.836679	0.098180	0.009459	382.2048	-1076.729040	-1076.774918
2	-267.602631	0.074599	0.007417	323.2675	-267.520615	-267.559418
3	-1256.442281	0.156831	0.015706	508.6912	-1256.269744	-1256.330804
4	-2333.304455	0.259172	0.024622	684.5496	-2333.020661	-2333.102830
5	-2065.675154	0.179807	0.017912	560.089	-2065.477435	-2065.544665
6	-3142.533530	0.281327	0.027412	776.5099	-3142.224791	-3142.317999
3'	-1523.282079	0.211567	0.020715	620.0313	-1523.049797	-1523.124222
4'	-2600.14471	0.313467	0.029102	781.0487	-2599.802142	-2599.895894
5'	-2332.514896	0.234445	0.02293	672.8726	-2332.257521	-2332.338289
6'	-3409.379482	0.336083	0.031553	852.576	-3409.011846	-3409.114184
1 core	-538.676802	0.050747	0.005804	290.1262	-538.620251	-538.6550761
3' core	-1217.144645	0.129456	0.01412	475.5408	-1217.001069	-1217.05815
4' core	-1755.838834	0.183802	0.019831	615.4366	-1755.635201	-1755.709075
5' core	-1488.218582	0.105764	0.012109	432.4629	-1488.100709	-1488.152619
6' core	-2026.914976	0.160236	0.017815	565.4366	0.067872	-2026.736926

Table S2. Thermodynamic parameters (in a.u.) for each species calculated at G3(MP2)-RAD//M062X/6-31G(d) level of theory in the gas phase at 42°C.

T=315.15 K	$E_{\text{CCSD(T)/6-31G(d)}}$	$E_{\text{R(O)MP2/6-31G(d)}}$	$E_{\text{R(O)MP2/G3MP2Large}}$	<i>HLC</i>	$E_{\text{G3(MP2)-RAD}}$	$G_{\text{G3(MP2)-RAD}}$	E_{onion}	G_{onion}
1	-1075.330475	-1075.236722	-1075.621914	-0.173403	- 1075.88907 0	-1075.827308	-1075.761310	-1075.699549
2	-266.976452	-266.918589	-267.225919	-0.135751	-267.419533	-267.376320	-267.419533	-267.376320
3	-1254.324846	-1254.191326	-1254.890678	-0.301216	- 1255.32541 3	-1255.213936		
4	-2329.673075	-2329.445398	-2330.535830	-0.474619	- 2331.23812 6	-2331.036501		
5	-2062.677594	-2062.508859	-2063.288837	-0.338868	-2063.79644	-2063.665951		
6	-3138.023992	-3137.761052	-3138.933726	-0.512271	- 3139.70893 7	-3139.493406		
3'		-1520.341705	-1521.308793	-0.432998			-1521.699228	-1521.541371
4'		-2595.597923	-2596.957855	-0.606401			-2597.488803	-2597.239987
5'		-2328.659451	-2329.707706	-0.470650			-2330.043513	-2329.866906
6'		-3403.918552	-3405.359594	-0.644053			-3405.836058	-3405.570760
1 core	-537.921817	-537.871106	-538.067506	-0.088686	-538.206903	-538.185177		
3' core	-266.976452	-266.918589	-267.225919	-0.135751	-267.419533	-267.376320		

4' core	-1215.137255	-1215.019796	-1215.667914	-0.272977	- 1216.05834 9	-1215.971855		
5' core	-1753.070410	-1752.901126	-1753.750580	-0.361663	- 1754.28152 7	-1754.151768		
6' core	-1486.081108	-1485.971213	-1486.511111	-0.225912	- 1486.84691 8	-1486.780956		

Table S3. Solvation energies for each species calculated at M062X/6-31G(d) level of theory.

Species	$\Delta G_{\text{solv}}(\text{THF})$	$\Delta G_{\text{solv}}(\text{DMSO})$	$\Delta G_{\text{solv}}(\text{DMF})$	$\Delta G_{\text{solv}}(\text{sulfolane})$	$\Delta G_{\text{solv}}(\text{DCM})$	$\Delta G_{\text{solv}}(\text{CPME})$
1	-0.009371	-0.008081	-0.009461	-0.005900	-0.010942	-0.007455
2	-0.005850	-0.005506	-0.006314	-0.003727	-0.005766	-0.002596
3	-0.014780	-0.014238	-0.015848	-0.011000	-0.015290	-0.009709
4	-0.018832	-0.017202	-0.019573	-0.012928	-0.020554	-0.014334
5	-0.017497	-0.015771	-0.018014	-0.012115	-0.019967	-0.014166
6	-0.024984	-0.022905	-0.025963	-0.017833	-0.028221	-0.020537
3'	-0.020472	-0.019520	-0.021854	-0.015320	-0.021700	-0.012756
4'	-0.026631	-0.025055	-0.028181	-0.019608	-0.029273	-0.019547
5'	-0.022518	-0.020444	-0.023356	-0.015834	-0.025332	-0.016070
6'	-0.029593	-0.026682	-0.030507	-0.020628	-0.033595	-0.022503

Table S4. Thermodynamic parameters (in a.u.) for each species calculated at G3(MP2)-RAD//M062X/6-31G(d) level of theory at 42°C in different solvents.

$G_{G3(MP2)-RAD}$	$G_{G3(MP2)-RAD(THF)}$	$G_{G3(MP2)-RAD(DMSO)}$	$G_{G3(MP2)-RAD(DMF)}$	$G_{G3(MP2)-RAD(sulfolane)}$	$G_{G3(MP2)-RAD(DCM)}$	$G_{G3(MP2)-RAD(CPME)}$
1	-1075.833433	-1075.832143	-1075.833523	-1075.829962	-1075.835004	-1075.831517
1 (ONIOM)	-1075.705673	-1075.704383	-1075.705763	-1075.702202	-1075.707244	-1075.703757
2	-267.378924	-267.378580	-267.379388	-267.376801	-267.378840	-267.375670
3	-1255.225470	-1255.224928	-1255.226538	-1255.221690	-1255.225980	-1255.220399
4	-2331.052087	-2331.050457	-2331.052828	-2331.046183	-2331.053809	-2331.047589
5	-2063.680202	-2063.678476	-2063.680719	-2063.674820	-2063.682672	-2063.676871
6	-3139.515144	-3139.513065	-3139.516123	-3139.507993	-3139.518381	-3139.510697
3'	-1521.558597	-1521.557645	-1521.559979	-1521.553445	-1521.559824	-1521.550881
4'	-2597.263372	-2597.261796	-2597.264921	-2597.256349	-2597.266014	-2597.256288
5'	-2329.886177	-2329.884104	-2329.887016	-2329.879494	-2329.888991	-2329.879730
6'	-3405.597106	-3405.594196	-3405.598020	-3405.588142	-3405.601109	-3405.590016

Appendix S2 Gaussian Archive Files

1.VC_dimer

```
1\1\GINC-R44\FOpt\UM062X\Gen\C4H7Cl2(2)\ROOT\18-Dec-2018\0\#M062X/gen
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11482978\C,-0.6838553987,-1.2331989778,1.9491256322\H,-1.7135185734,-1
.2773489346,1.5765094208\H,-0.139954438,-2.0911074605,1.5300810864\C,-
0.7159508246,-1.3271415697,3.4300951755\Cl,0.7832877393,-1.5047231583,
4.2759846532\H,-1.5264042941,-0.9488814108,4.0382763169\H,-1.003184534
9,-0.0023460482,-0.5226547661\H,0.495785985,0.9545200025,-0.4944051212
\H,0.5756901238,-0.8186319393,-0.4857691088\Version=ES64L-G09RevE.01\
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e-09\RMSF=8.426e-06\Dipole=-0.088587,-0.6894743,-0.8895111\Quadrupole=
1.4676996,-3.0388898,1.5711903,1.9893624,-2.1657991,2.0083596\PG=C01 [
X(C4H7Cl2)]\@
```

2.LG_r.a1

```
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8622509245,3.2882667661\H,1.1424047915,-1.8226712894,3.7987547135\H,2.
0599591757,-0.3824180397,3.2618933671\H,0.3729794916,-0.2063819264,3.8
047988807\C,0.0145772053,-0.4361072393,-0.1553209435\H,-0.1360601434,0
.3524550677,-0.8793780262\H,-0.1775142701,-1.4677026563,-0.4175655641\
O,0.6230105099,-1.1516788086,1.967218372\C,0.477739082,-0.0760833251,1
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adrupole=-0.4935495,-4.2381841,4.7317336,-0.5013708,1.7969973,-0.51602
91\PG=C01 [X(C3H5O2)]\@
```

3.raft.a1b2

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rahydrofuran) maxdisk=1073741824\raft.a1b2.thf.freq\0,1\C,0.98640852
04,-0.8540548981,3.2399603272\H,0.7949951575,-1.8005043823,3.743503159
6\H,2.0540338503,-0.6237626614,3.254336039\H,0.4322254229,-0.046484966
4,3.7231945132\C,0.1482752635,-0.2826007415,-0.28535583\H,-0.936752118
7,-0.1274463064,-0.2723895452\H,0.3386623234,-1.32597064,-0.5415244111
\C,4.445460311,0.9504673926,-2.8405181014\H,5.0040000937,1.1121283067,
-1.9144693273\H,4.6124918446,-0.0773851879,-3.174406777\C,4.7900028468
,1.9643732019,-3.9047562924\H,5.8510737411,1.874542308,-4.152918044\H,
4.2054871226,1.7910787153,-4.8121122374\H,4.6015107444,2.9808378143,-3
.5495559202\O,0.5379615501,-1.0325297071,1.8915041168\C,0.6904690071,0
.0303452161,1.0993597404\O,1.142737153,1.087772368,1.4577894951\S,0.76
96762014,0.8151941293,-1.567680214\C,2.4703969619,0.344589133,-1.63817
15257\S,3.2008937101,-0.8273650044,-0.7432638389\O,3.0373002927,1.1077
989102,-2.5516553268\Version=ES64L-G09RevE.01\State=1-A\HF=-1256.4570
609\RMSD=5.944e-09\RMSF=1.029e-05\Dipole=-0.0604474,-0.314027,-0.25735
25\Quadrupole=3.6746582,-8.0362212,4.361563,4.8417842,-6.9988369,-5.17
40542\PG=C01 [X(C6H10O3S2)]\@

4.raft_VC_dimer.a1b2c2f2g3

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714672,4.6905959758\H,-2.5516376856,1.5100713817,4.5855505897\H,-1.858
0561372,3.1153122931,4.940345977\C,-1.4123193309,2.8041608972,0.941116
4331\H,-1.1684854364,3.8667686399,0.8338162817\H,-2.4140153622,2.64839
36069,0.5383945527\C,-2.7771095606,-0.8998428034,0.8198382636\H,-3.747
6899236,-1.0257285191,0.3360920095\H,-2.2089872542,-1.8289924839,0.710
6414983\C,-2.9262275126,-0.4991043093,2.2731523658\H,-3.4235960705,-1.
2992413807,2.8302424406\H,-1.9447550587,-0.3238803,2.7254236235\H,-3.5
283321728,0.4114640071,2.3589152922\O,-2.5359100553,2.8464753413,2.989
7527776\C,-1.3941162443,2.4577628021,2.4186347778\O,-0.488092164,1.931
5685085,3.0195227011\S,-0.1879554262,1.8959216372,-0.0345193409\C,-0.7
921269451,0.2604250825,0.2068858973\S,0.2542012234,-1.0534143875,-0.35
48065747\O,-2.1308141163,0.144278062,0.0680099651\C,1.1409665748,-1.54
13104009,1.1631520675\H,1.9025851115,-2.2399425205,0.8108560335\C,1.76
15998148,-0.3678374196,1.9035053562\H,2.4114357129,0.1597547146,1.1948
621387\H,0.9716712614,0.327956912,2.2115870918\C,2.5631003435,-0.72232
75669,3.14676358\H,1.9468118063,-1.2674383672,3.8628096231\C,3.1667668
884,0.5118717779,3.7887463513\H,3.7320987033,0.2507591204,4.6863349777

\H,3.8302075111,1.0291555829,3.089414075\H,2.3576148986,1.1939843022,4
.0707710043\Cl,3.9007968075,-1.8904787619,2.7172965196\Cl,0.0910092066
, -2.5128530128,2.2845796156\Version=ES64L-G09RevE.01\State=2-A\HF=-23
33.3232872\S2=0.754482\S2-1=0.\S2A=0.750017\RMSD=4.079e-09\RMSF=8.509e
-06\Dipole=-1.7782944,1.6084017,1.0498896\Quadrupole=0.591786,0.424375
5,-1.0161615,1.7843854,-4.7938802,4.6154755\PG=C01 [X(C10H17Cl2O3S2)]\
\@

5.raft_noLG_VC_dimer.a1c2

1\1\GINC-R104\FOpt\RM062X\Gen\C7H12Cl2O1S2\ROOT\20-Dec-2018\0\#M062X/
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=tetrahydrofuran) maxdisk=1610612736\raft_noLG_VC_dimer.a1c2.freq\0,
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3,2.3898934337\C,-1.811812286,0.4182038798,2.9615892784\S,1.1202177955
,0.9472491035,-0.252237976\C,-1.8453287697,-0.2620236426,4.3256070381\
C,-3.2265114402,-0.3662595972,4.9590038087\Cl,-4.3481259659,-1.2653397
306,3.837597256\Cl,-2.5047262395,2.0857740858,3.0509448283\C,-3.176516
5053,-1.0817363823,6.2950162499\H,-2.4187644466,-0.114612254,2.2308672
919\H,-1.429409928,-1.2695328561,4.2076272766\H,-1.2055134455,0.285633
7286,5.0287659993\H,-3.67819465,0.6207990304,5.0658699078\H,-4.1734454
733,-1.1535716203,6.7354556162\H,-2.7648602275,-2.0889223616,6.1824883
803\H,-2.5356194749,-0.5152378625,6.9787349165\O,-1.4842960029,0.84547
1701,0.2660185437\C,-1.7816256084,1.129548676,-1.1248702368\H,-1.31516
14496,2.0846698558,-1.3798730533\H,-1.329900626,0.3422976418,-1.734155
2376\C,-3.2854410398,1.1681937414,-1.2452771063\H,-3.5541911166,1.3855
377343,-2.28257261\H,-3.7237417285,0.2058062831,-0.967903113\H,-3.7063
383874,1.9484343526,-0.6056575097\Version=ES64L-G09RevE.01\State=1-A\
HF=-2065.6926511\RMSD=7.919e-09\RMSF=7.841e-06\Dipole=-1.0407919,-0.33
96169,0.6122352\Quadrupole=-13.3027759,-2.3356725,15.6384484,-3.811999
1,7.7600731,-2.7450408\PG=C01 [X(C7H12Cl2O1S2)]\
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6.raft_noLG_VC2_dimer.a2b3c3e3

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.freq\0,2\C,-0.3311908291,-0.9092466186,-0.2744504713\S,-1.2800330258
, -0.9997019739,-1.738836829\C,-0.3570621268,0.1512540089,-2.8208591801
\S,-0.939076,-0.0006833916,1.0886996179\C,-0.8559253865,-0.0111187268,

-4.2489403661\C,-0.1563233725,0.8599080608,-5.2837469832\Cl,1.63068550
72,0.4930944883,-5.2797074757\Cl,-0.5237186503,1.8636529442,-2.2564165
242\C,-0.7076760427,0.6317910621,-6.6777053036\H,0.707261709,-0.071032
739,-2.7357811605\H,-0.7338263384,-1.0644245371,-4.5288454237\H,-1.926
495285,0.2252083182,-4.2903601413\H,-0.2212490766,1.9137764184,-5.0090
839254\H,-0.1904449006,1.257452587,-7.4085223183\H,-0.6026124126,-0.41
68632573,-6.9710375562\H,-1.7709935092,0.8934386516,-6.6877810796\C,-0
.314696274,-1.0467363703,2.4381937324\C,-0.3414195669,-0.2604270072,3.
7411186073\Cl,-1.2747558558,-2.5806442235,2.5845248144\H,0.6965190947,
-1.3616018154,2.1789722998\C,0.1493486004,-1.0182247622,4.9674284445\H
,0.2770138019,0.6340324528,3.6016774265\H,-1.3667093102,0.069789286,3.
9508411852\C,0.1278326918,-0.1507330302,6.2109495149\H,-0.4355602949,-
1.9263299118,5.1195337405\Cl,1.8502215338,-1.612997611,4.6810550613\H,
0.4855649798,-0.7067677213,7.0804011752\H,0.7513409682,0.7381097094,6.
077204242\H,-0.901535131,0.1695495702,6.4037719822\O,1.0063851285,-1.0
869161487,-0.3004895549\C,1.509126379,-2.2831104436,-0.9324210558\H,2.
5917075902,-2.1465619426,-0.9297464105\H,1.1656529574,-2.3189446123,-1
.9721026117\C,1.0995295727,-3.5251308089,-0.1701460676\H,1.5533064203,
-4.4053025324,-0.6354140281\H,1.438904055,-3.4700456704,0.8691957381\H
,0.0126213986,-3.6518517019,-0.1778381156\Version=ES64L-G09RevE.01\St
ate=2-A\HF=-3142.5585139\S2=0.755699\S2-1=0.\S2A=0.750027\RMSD=7.053e-
09\RMSF=1.878e-06\Dipole=-0.5567393,-0.1930929,-0.489926\Quadrupole=-9
.564475,-6.6316786,16.1961535,-4.6142627,2.6779097,7.3856437\PG=C01 [X
(C11H19Cl4O1S2)]\@

raft2.M062X (3')

1\1\GINC-R3294\FOpt\RM062X\Gen\C11H12O4S2\ROOT\11-Nov-2019\0\#\# M062X/
Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=214748364
8\raft2.M062X\0,1\C,-3.9664852499,-0.7885536292,0.9890971477\H,-4.83
55571822,-1.2545890252,0.5282013389\H,-3.3251408075,-1.5399288095,1.45
45780529\H,-4.2715063377,-0.0615011262,1.7446587042\C,-1.4885556669,1.
127432353,-0.9112196458\H,-1.9899106556,2.0782436779,-1.1209697167\H,-
1.6074267664,0.4743980817,-1.7772043067\O,-3.2652511069,-0.1393292566,
-0.0724797208\C,-2.1450289853,0.4893163463,0.3045398837\O,-1.756789795
2,0.5635905978,1.4390796423\S,0.2428307018,1.5394729631,-0.6516680562\
C,0.9442716099,-0.073476182,-0.5444860465\S,0.1694698901,-1.503724511,
-0.6842899405\O,2.2552006162,0.1131248298,-0.3311330239\C,3.0937269733
, -0.9965559456,-0.1830691387\C,3.3080103787,-1.5163905385,1.078902737\
C,3.7417082929,-1.5069007379,-1.3014057049\C,4.1950236156,-2.580018422
,1.240680611\H,2.7821401467,-1.0940034042,1.9285969232\C,4.623419951,-
2.562429835,-1.1432575976\H,3.5487703896,-1.0748057429,-2.2775209411\C
,4.8533963327,-3.1049254544,0.1270485272\H,4.3594394489,-2.9844161914,
2.2318680604\H,5.1499261402,-2.9901269203,-1.9892838893\O,5.7354854099
, -4.135992965,0.1734611283\C,5.9893082584,-4.7199950596,1.4319890091\H
,6.7071075884,-5.5204577167,1.2547095861\H,6.4207481987,-3.9918405448,
2.1295830344\H,5.0747766103,-5.1400838317,1.8677683424\Version=ES64L-
G09RevE.01\State=1-A\HF=-1523.2820789\RMSD=8.795e-09\RMSF=3.384e-06\Di

pole=-0.086314,-0.4170455,0.1885129\Quadrupole=7.4783173,-3.8694025,-3.6089148,-7.2241283,4.6837612,-7.9885161\PG=C01 [X(C11H12O4S2)]\@

raft2_noLG_VC_dimer.M062X (5')

1\1\GINC-R2976\FOpt\RM062X\Gen\C12H14Cl2O2S2\ROOT\11-Nov-2019\0\#\ M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2147483648\raft2_noLG_VC_dimer.M062X\0,1\C,-2.2132051177,-0.40920601,-0.5756243185\S,-0.6942317267,-1.312050479,-0.4195813766\C,-1.0069455467,-2.7627428943,-1.4524792404\S,-3.5022961893,-0.7632546681,-1.5009223351\C,0.3384918806,-3.3501009723,-1.8682843324\C,0.2430466172,-4.5591277004,-2.7914075778\C1,-0.6182853132,-4.0906632494,-4.313391764\C1,-1.9947605279,-3.9976906353,-0.5898355978\C,1.6153912633,-5.1093046564,-3.1400226979\H,-1.599899854,-2.4537788309,-2.3147895359\H,0.9121279112,-2.5630957128,-2.3716694081\H,0.896161876,-3.6528367388,-0.9730514768\H,-0.3802194648,-5.3315781528,-2.337888533\H,1.5295229036,-5.9638818564,-3.8138718633\H,2.2262153718,-4.3430314297,-3.6256853515\H,2.1219338909,-5.4352262826,-2.2256135974\O,-2.0653999454,0.6463086469,0.2394284875\C,-3.1018192292,1.581151571,0.3476260175\C,-3.1101048073,2.6844893091,-0.4972073007\C,-4.0541816556,1.4161054619,1.3344649968\C,-4.0996502399,3.6399965796,-0.342551358\H,-2.3474255767,2.7816752315,-1.2624755966\C,-5.0522249988,2.3769633313,1.4919151243\H,-4.0172806001,0.540807294,1.9742217285\C,-5.0758529243,3.4908665341,0.6506639246\H,-4.1432196186,4.5159103205,-0.9802585049\H,-5.7971246415,2.2429794988,2.2665949196\O,-5.9994789596,4.482817858,0.7182703957\C,-7.0105160062,4.3666018317,1.6952227734\H,-7.6449028039,5.2449142114,1.5796808691\H,-7.6096758799,3.4610367181,1.5417721917\H,-6.587193087,4.3534968716,2.706901338\Version=ES64L-G09RevE.01\State=1-A\HF=-2332.5148959\RMSD=5.606e-09\RMSF=5.725e-06\Dipole=0.3470777,0.4517709,0.8604846\Quadrupole=7.5721737,-0.4188353,-7.1533384,-13.8636983,-10.2132793,2.5662311\PG=C01 [X(C12H14Cl2O2S2)]\@

raft2_VC_dimer.M062X (4')

1\1\GINC-R2216\FOpt\UM062X\Gen\C15H19Cl2O4S2(2)\ROOT\15-Nov-2019\0\#\ M062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=2684354560\raft2_VC_dimer.M062X\0,2\C,3.7347843219,0.5367180167,-2.0401245824\H,4.6195852753,-0.0287608499,-2.3273697426\H,2.8378318258,0.1059342153,-2.4916593087\H,3.8274607025,1.5819178361,-2.34279793\C,2.6658616083,0.9130611048,1.4571023142\H,3.0859977248,1.8101142816,1.9215521696\H,3.2836248881,0.0529949826,1.7128597404\O,3.6644316829,0.4390367582,-0.6140393636\C,2.6466102279,1.0995186076,-0.0523845637\O,1.8410250583,1.7528140857,-0.663636527\S,0.9986217259,0.735592208,2.1562406003\C,0.361334137,-0.4657600459,1.0587822951\S,-1.2480526847,-1.0775851325,1.3244968894\O,1.3037495322,-1.214112345,0.4200549678\C,-0.9708842043,-2.352664767,2.6131886304\H,-0.3116298956,-1.9404338306,3.3783136849\C,-2.3234137093,-2.7435765558,3.1943202253\H,-2.8030396198,-1.8336208811,3.5741234614\H,-2.9534800362,-3.1453913651,2.3903735461\C,-2.2709782692,-3.7800142132,4.3103604206\H,-1.7449842061,-4.6732474448,3.9691709838\C,-3.6580093213,-4.1313099091,4.8202325613\H,-3.600308247,-4.8646520932,5.6269835851\H,-4.1679406408,-3.2396343321,5.1957263155\H,-4.2502326687,-4.5564382142,4.0032227352\C1,-1.2740035299,-3.1438382986,5.6833829219\C1,-0.1198395696,-3.8015141293,1.9561600528\C,1.1194076154,-1.5203126607,-0.9200960588\C,1.8339407413,-2.6047666901,-1.4031595573\C,0.3277336974,-0.7479750099,-1.7691850636\C,1.7699818573,-2.9337839634,-2.7560736591\H,2.4399303744,-3.1826294948,-0.7137365464\C,0.2565215342,-1.0832067386,-3.1126723074\H,-0.1955330747,0.1205708714,-1.3840120905\C,0.9745592021,-2.1734858434,-3.615656058\H,2.3352199534,-3.7836368855,-3.1193399255\H,-0.3482286706,-0.5027397558,-3.800989915\O,0.8355966232,-2.4103977226,-4.9483245098\C,1.5326112711,-3.5106172351,-5.48

62526415\H,1.2173205538,-4.4510426163,-5.0177473417\H,1.2880619048,-3.5354650383,-6.5479919498\H,2.6170653081,-3.3949639061,-5.3657994587\Version=ES64L-G09RevE.01\State=2-A\HF=-2600.1447105\S2=0.754992\S2-1=0.\S2A=0.750021\RMSD=9.134e-09\RMSF=3.520e-06\Dipole=0.4865898,-0.7534125,-0.7778712\Quadrupole=7.710513,-5.2888993,-2.4216138,5.6490081,-9.5927614,6.7815166\PG=C01 [X(C15H19C12O4S2)]\@

raft2_noLG_VC2_dimer.M062X (6')

1\1\GINC-R2446\FOpt\UM062X\Gen\C16H21C14O2S2(2)\ROOT\15-Nov-2019\0\#\M062X\Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=3221225472\raft2_noLG_VC2_dimer.M062X\0,2\C,-0.1042344127,0.1044991612,-0.5824742858\S,-1.6177021423,-0.1332350296,-1.425060093\C,-2.7241383067,-0.457282074,-0.0102614045\S,1.1203459695,-1.1305602213,-0.6753357098\C,-4.1680462339,-0.4012188496,-0.4869897586\C,-5.2038925309,-0.5467866267,0.6219949925\C1,-4.9873290735,0.7871312989,1.8310039532\C1,-2.3629750753,-2.0378528261,0.7785299503\C,-6.6221717068,-0.5048861406,0.0804742906\H,-2.5379764355,0.3005204369,0.7511216809\H,-4.3204509561,0.560181521,-0.9919174515\H,-4.3388153371,-1.1999512062,-1.2196385738\H,-5.028781924,-1.4672520038,1.1819140924\H,-7.3493098695,-0.596623329,0.8895774669\H,-6.8049686307,0.4351771074,-0.4476727825\H,-6.7703670836,-1.3348757968,-0.6181767954\C,2.5912168461,-0.1044263372,-0.3804190504\C,3.7889823793,-1.0216685349,-0.1718385168\C1,2.8961381659,1.0430138086,-1.7453347264\H,2.4099776372,0.5222011397,0.4929697534\C,5.1000176772,-0.3067999473,0.1326798617\H,3.5528644527,-1.7013419729,0.6556093488\H,3.9370883309,-1.6284901659,-1.0741472495\C,6.2472394477,-1.2864437164,0.3101706907\H,5.3256988214,0.4156049212,-0.6536492268\C1,4.9185660989,0.6803923617,1.6402346126\H,7.1752621448,-0.7586455365,0.5381833506\H,6.0347484777,-1.9851265256,1.1242640457\H,6.3875260383,-1.8563944346,-0.614196418\O,-0.0802558417,0.8590069829,0.5534324245\C,-0.559234923,2.1641918897,0.4765409853\C,-0.2771289237,2.9881594,-0.6013382789\C,-1.3071727764,2.6256680513,1.5568776853\C,-0.7525928595,4.298839547,-0.6075907303\H,0.3141948137,2.6086802223,-1.4289376723\C,-1.7761140871,3.928813805,1.5524183673\H,-1.5096140389,1.9575946397,2.3884104674\C,-1.503238385,4.7725829819,0.4697709682\H,-0.5256520688,4.9349646078,-1.4545491277\H,-2.3629171588,4.3184554122,2.376905387\O,-2.0104676385,6.0302268334,0.5596848285\C,-1.7503281587,6.9131025118,-0.5082382182\H,-2.2322503378,7.8549273121,-0.2469250378\H,-0.6735273394,7.0781132575,-0.6362503408\H,-2.1717470456,6.537061064,-1.4485907555\Version=ES64L-G09RevE.01\State=2-A\HF=-3409.3794815\S2=0.755594\S2-1=0.\S2A=0.750025\RMSD=8.082e-09\RMSF=3.544e-06\Dipole=-0.2730615,0.1358377,-0.9789395\Quadrupole=7.8400437,3.3701286,-11.2101723,-4.6268506,1.3797471,-4.7047531\PG=C01 [X(C16H21C14O2S2)]\@

VC_dimer_core.M062X (1 core)

1\1\GINC-R2450\FOpt\UM062X\Gen\C2H4C11(2)\ROOT\13-Nov-2019\0\#\M062X\Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=671088640\VC_dimer_core.M062X\0,2\C,-0.1196921373,0.7545315047,0.8485903188\H,0.4165433689,0.6674311247,1.7974484933\H,-0.4232892397,1.7973504001,0.7126799548\C,-1.2998530598,-0.145864343,0.8531811979\C1,-2.4314065715,-0.0184127185,-0.4427922678\H,-1.3018009031,-1.1091297737,1.3453498758\H,0.5831492225,0.5096774558,0.0388935371\Version=ES64L-G09RevE.01\State=2-A\HF=-538.6768023\S2=0.755026\S2-1=0.\S2A=0.750021\RMSD=9.150e-09\RMSF=1.388e-05\Dipole=0.5655158,-0.0336603,0.357667\Quadrupole=-0.0683207,0.2197598,-0.1514391,0.136322,0.5892913,-0.556556\PG=C01 [X(C2H4C11)]\@

raft2_core.M062X (3' core)

1\1\GINC-R1996\FOpt\RM062X\Gen\C5H8O3S2\ROOT\13-Nov-2019\0\#\M062X\Ge

n 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073741824\
\raft2_core.M062X\0,1\C,4.7886495416,2.4447854911,-0.1599890431\H,5.3
57477479,2.9134745237,-0.9610172815\H,3.863209636,2.9925336623,0.02989
86761\H,5.375399637,2.4050761908,0.760165475\C,3.5151680964,-0.9843706
275,-0.3617758323\H,4.4054335052,-1.6047056346,-0.2135477858\H,3.33719
48108,-0.8860994011,-1.4337934499\O,4.4891674834,1.1250642234,-0.61708
55569\C,3.7740446076,0.388368902,0.2422878515\O,3.4346789955,0.7567732
319,1.3341614866\S,2.169272792,-1.8732609836,0.4344838143\C,0.79168156
38,-0.8919347118,-0.065220265\S,0.8205227785,0.4367880433,-1.025531190
4\O,-0.2833816294,-1.4436091583,0.4821662213\C,-1.555048281,-0.8378928
572,0.2461069235\H,-1.778221101,-0.8374947148,-0.8229550472\H,-2.26619
03527,-1.4524955104,0.7949477124\H,-1.5544629329,0.1894303509,0.616406
6716\Version=ES64L-G09RevE.01\State=1-A\HF=-1217.1446453\RMSD=7.051e-
09\RMSF=4.246e-06\Dipole=0.0220376,-0.0426796,-0.35047\Quadrupole=9.02
07417,-1.0635074,-7.9572343,2.8365168,-2.289096,0.0740702\PG=C01 [X(C5
H8O3S2)]\@

raft2_noLG_VC_dimer_core.M062X (5' core)
1\1\GINC-R2422\FOpt\RM062X\Gen\C4H7C11O1S2\ROOT\13-Nov-2019\0\#\ M062X
/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=10737418
24\raft2_noLG_VC_dimer_core.M062X\0,1\C,-0.2349427394,-0.1390207037,
0.4011233866\S,1.1986229016,-0.7337643365,1.2573844696\C,2.5385280696,
-0.2821107887,0.1279792051\S,-0.2886081253,0.7105526293,-0.9946898766\
C,3.8404362746,-0.2263712985,0.9116327242\C1,2.6958074364,-1.448078653
, -1.2351266869\H,2.2852801904,0.6753013515,-0.328202445\H,3.7710578756
,0.5344648282,1.6936025634\H,4.0618721198,-1.1928385184,1.3716121059\O
, -1.2733016082,-0.5141575201,1.1371303191\C,-2.5841827837,-0.147494708
7,0.7026298249\H,-2.7862481227,-0.578578173,-0.2800718021\H,-3.2548590
402,-0.5562417255,1.4560310434\H,-2.670479389,0.9396916593,0.646123119
3\H,4.6584632105,0.0291729677,0.2351439392\Version=ES64L-G09RevE.01\St
ate=1-A\HF=-1488.218582\RMSD=5.461e-09\RMSF=7.542e-06\Dipole=-0.31733
45,0.3518001,0.7828679\Quadrupole=8.6853314,-3.7618762,-4.9234552,1.83
08899,0.4049592,0.5491541\PG=C01 [X(C4H7C11O1S2)]\@

raft2_VC_dimer_core.M062X (4' core)
1\1\GINC-R1518\FOpt\UM062X\Gen\C7H12C11O3S2(2)\ROOT\15-Nov-2019\0\#\ M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1610
612736\raft2_VC_dimer_core.M062X\0,2\C,-4.5427224772,2.6129009368,-0
.6943629229\H,-5.1894296707,2.9093500902,-1.5182658696\H,-4.6018670992
,1.5353293515,-0.52565002\H,-4.823913599,3.1313250495,0.2245793221\C,-
0.9166085448,3.122123898,-0.7350195024\H,-0.9025663931,4.211545061,-0.
8329592843\H,-0.802271733,2.6941813842,-1.7325421563\O,-3.2195561067,2
.9794812351,-1.0873824078\C,-2.2667429495,2.6933615688,-0.1859381244\O
, -2.4858140557,2.1756964545,0.8771448965\S,0.4847611166,2.6770623375,0
.3156977686\C,0.2016433688,0.9527936585,0.4621103152\S,1.3216744147,0.
0241840885,1.4191678504\O,-0.5357918621,0.4059374671,-0.5325685708\C,2
.6880834734,-0.3145630302,0.2398768527\H,2.9119685159,0.6084473851,-0.
2962006525\C,3.8876491191,-0.8358001717,1.0102142299\H,4.220364598,-0.
0806352998,1.7275860432\H,3.6267684276,-1.7495497135,1.5509721387\C1,2
.2076397291,-1.5063480338,-1.0296989244\C,-1.3216769099,-0.7240667527,
-0.1588056363\H,4.705650212,-1.0610944217,0.3222885009\H,-0.6781909376
, -1.5598120229,0.1293407144\H,-1.9862263554,-0.4505252077,0.6664888363
\H,-1.8987086414,-0.9896927623,-1.044794907\Version=ES64L-G09RevE.01\
State=2-A\HF=-1755.838834\S2=0.755083\S2-1=0.\S2A=0.750022\RMSD=8.895e
-09\RMSF=1.848e-06\Dipole=-0.5574641,0.3658707,-0.5238512\Quadrupole=9
.7286552,-1.7968841,-7.9317711,-1.0818667,5.2770137,-3.8589296\PG=C01
[X(C7H12C11O3S2)]\@

raft2_noLG_VC2_dimer_core.M062X (6' core)
1\1\GINC-R2752\FOpt\UM062X\Gen\C6H11Cl2O1S2(2)\ROOT\15-Nov-2019\0\#\ M
062X/Gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1073
741824\raft2_noLG_VC2_dimer_core.M062X\0,2\C,-0.31742695,-0.70365560
62,0.6610976966\S,1.1301494562,-1.1301607711,1.5386821921\C,2.17906342
11,-1.7783692909,0.1845053952\S,-1.6700201495,-1.8029267223,0.66689891
19\C,3.612130195,-1.8921669538,0.6718551341\C1,1.5955513039,-3.3747829
074,-0.4156885889\H,2.0844722492,-1.0995824433,-0.6639096393\H,3.97876
44171,-0.907747086,0.9758957022\H,3.6733227605,-2.5731887451,1.5247893
165\C,-2.9847327489,-0.65759812,0.1545033371\C,-4.2904918465,-1.422268
8959,0.0316664854\C1,-3.1758421609,0.720826569,1.3097070034\H,-2.68686
18791,-0.197431637,-0.7861324026\H,-4.1815818441,-2.2221200411,-0.7063
210991\H,-4.5725480394,-1.8594264114,0.9926537371\O,-0.2539674178,0.14
65640586,-0.3957952647\C,0.2254708587,1.4574858997,-0.0957818852\H,-5.
0851277996,-0.7472107657,-0.2926488253\H,4.2479497526,-2.278688628,-0.
1276155051\H,1.2649438265,1.423370882,0.2448243321\H,0.1561359013,2.02
10578261,-1.0259419381\H,-0.4007523961,1.9153108599,0.6754584646\Version=ES64L-G09RevE.01\State=2-A\HF=-2026.9149763\S2=0.755576\S2-1=0.\S2
A=0.750025\RMSD=4.750e-09\RMSF=4.946e-06\Dipole=0.3793384,0.7584622,-0
.6438775\Quadrupole=7.3911731,-3.1785652,-4.2126079,4.8684699,2.877629
8,-2.6869895\PG=C01 [X(C6H11Cl2O1S2)]\@