ESI for manuscript:

Evaluation of the Solvent Competitive Binding in Halogen and Chalcogen Bonding: A Theoretical Theory Study for Supramolecular Applications

by

Eric Miguens,[a] Mariana Rocha[b] and Antonio Frontera*[,a]

a. Departament de Química, Universitat de les Illes Balears, Crta de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), Spain. E-mail: toni.frontera@uib.es.

b. INBIOFAL (CONICET – UNT), Instituto de Química Orgánica. Facultad de Bioquímica, Química y Farmacia, Universidad Nacional de Tucumán, Ayacucho 471, San Miguel de Tucumán, Argentina

Table of Contents

Table S1. Interaction free energies (ΔG, kcal/mol) for complexes **1**, **2**, **3** and **4** with the solvents.

	1	**2**	**3**	**4**
water	4.8	3.7	5.5	3.8
DMSO	6.7	3.5	5.9	2.8
acetonitrile	5.9	4.6	6.2	5.0
DMF	6.7	5.0	7.0	4.4
methanol	6.3	4.9	6.7	5.2
acetone	5.2	5.1	7.0	4.6
dichloromethane	8.1	7.1	7.9	8.7
trichloromethane	8.1	7.5	8.0	8.9
diethylether	6.9	5.6	7.3	6.1

Cartesian Coordinates

acetone
6 0.005470 0.177589 -0.000001
8 -0.022251 1.382664 0.000000
6 -1.273589 -0.627724 0.000000
1 -1.861003 -0.352860 -0.878720
1 -1.103308 -1.704419 -0.000042
1 -1.860960 -0.352925 0.878768
6 1.297535 -0.591793 0.000000
1 1.340131 -1.244733 0.877286
1 1.340137 -1.244722 -0.877293
1 2.146510 0.089916 0.000007
acetonitrile
6 0.000000 0.000000 -1.171282
1 0.000000 1.024579 -1.546520
1 -0.887311 -0.512289 -1.546520
1 0.887311 -0.512289 -1.546520
6 0.000000 0.000000 0.278763
7 0.000000 0.000000 1.427811
diethylether
6 -2.363764 0.408681 0.000025
1 -3.292144 -0.166709 -0.000031
1 -2.351793 1.048227 -0.884665
1 -2.351833 1.048129 0.884798
6 -1.171632 -0.514488 -0.000062
1 -1.189862 -1.169892 0.885449
1 -1.189858 -1.169759 -0.885677
8 0.000000 0.261210 0.000013
6 1.171632 -0.514488 0.000064
1 1.189847 -1.169902 -0.885441
1 1.189872 -1.169749 0.885685
6 2.363764 0.408681 -0.000034
1 2.351814 1.048265 0.884633
1 3.292144 -0.166708 0.000018
1 2.351812 1.048090 -0.884829
dmf
6 -0.858477 -0.641475 -0.000117
1 -0.751216 -1.743239 -0.000440
8 -1.938086 -0.094282 0.000344
7 0.343077 -0.019206 -0.001202
6 0.420156 1.418584 0.000110
1 0.952117 1.776089 0.887804
1 0.950124 1.777973 -0.887994
1 -0.592838 1.817083 0.001624
6 1.576379 -0.755544 0.000335
1 1.366248 -1.826129 0.003690
1 2.174987 -0.523910 -0.887338
1 2.175371 -0.518563 0.886341
dmso
16 -0.000054 0.233174 -0.437275

8 -0.000159 1.467230 0.382051
6 -1.340809 -0.797383 0.180043
1 -2.269859 -0.280747 -0.060952
1 -1.320174 -1.771514 -0.311957
1 -1.243372 -0.899172 1.262551
6 1.341054 -0.797121 0.180006
1 1.241493 -0.901160 1.262253
1 1.322623 -1.770347 -0.314080
1 2.269960 -0.278658 -0.058108
methanol
6 0.658759 -0.020111 0.000000
1 1.081952 0.985069 -0.000065
1 1.026942 -0.543940 0.891345
1 1.026931 -0.544049 -0.891284
8 -0.743678 0.121954 0.000000
1 -1.138955 -0.752043 0.000001
water
8 0.000000 0.000000 0.116716
1 0.000000 0.761619 -0.466862
1 0.000000 -0.761619 -0.466862
cf3br
6 0.000000 0.000000 -0.814144
9 0.000000 1.240417 -1.268962
9 -1.074233 -0.620209 -1.268962
9 1.074233 -0.620209 -1.268962
35 0.000000 0.000000 1.118481
cf3i
6 0.000000 0.000000 -1.180517
9 0.000000 1.241057 -1.641125
9 -1.074787 -0.620529 -1.641125
9 1.074787 -0.620529 -1.641125
53 0.000000 0.000000 0.969688
se(cf3)2
34 0.000004 1.022359 -0.000014
6 1.470206 -0.292109 -0.000002
6 -1.470208 -0.292101 0.000012
9 1.456335 -1.075900 1.069920
9 2.601186 0.409986 0.004256
9 1.461169 -1.070477 -1.073911
9 -1.456250 -1.076035 -1.069829
9 -1.461269 -1.070335 1.073995
9 -2.601186 0.409990 -0.004385
te(cf3)2
6 1.580477 -0.523012 -0.000025
6 -1.580477 -0.523011 0.000009
9 1.540400 -1.305940 1.073002
9 2.747918 0.125374 -0.000272
9 1.540040 -1.306311 -1.072710
9 -1.540554 -1.305700 -1.073181
9 -1.539887 -1.306550 1.072531
9 -2.747920 0.125374 0.000644

52 0.000001 0.981537 -0.000001
cf3br_acetone
6 2.395255 0.116353 -0.003360
9 2.900497 0.017292 1.217864
9 2.596555 1.353190 -0.437987
9 3.053776 -0.716056 -0.796359
35 0.513178 -0.299394 0.004970
6 -3.281298 -0.002544 0.000275
8 -2.407223 -0.836742 0.008909
6 -4.734818 -0.389689 -0.011230
1 -5.274230 0.120050 0.791628
1 -5.190387 -0.066910 -0.952308
1 -4.837937 -1.468094 0.092167
6 -2.979147 1.470891 0.002744
1 -3.526792 1.976823 -0.796680
1 -3.321345 1.908429 0.945607
1 -1.910154 1.642520 -0.107858
cf3br_acn
6 2.189675 0.000205 0.000042
9 2.657118 0.105000 1.236329
9 2.656935 1.018653 -0.708692
9 2.657568 -1.122619 -0.527424
35 0.265487 -0.000345 -0.000047
6 -4.002375 -0.000005 -0.000099
7 -2.854152 -0.000517 -0.000344
6 -5.451184 0.000532 0.000245
1 -5.825189 -0.932864 -0.423208
1 -5.824459 0.100624 1.020563
1 -5.824608 0.834229 -0.596343
cf3br_diethylether
6 2.415513 0.000005 0.092360
9 2.781647 1.077329 0.770233
9 3.056786 -0.005422 -1.065722
9 2.780251 -1.071888 0.779536
8 -2.484775 -0.000019 -0.193117
6 -2.767377 -1.174721 0.533254
1 -3.816324 -1.159215 0.866073
6 -2.767513 1.174664 0.533234
1 -2.140507 1.215904 1.437501
1 -3.816497 1.159111 0.865936
6 -2.509334 2.368820 -0.349644
1 -2.734238 3.292441 0.187878
1 -1.464138 2.399348 -0.662961
1 -3.134920 2.325510 -1.243157
6 -2.509241 -2.368855 -0.349668
1 -2.733907 -3.292499 0.187912
1 -3.135012 -2.325639 -1.243054
1 -1.464104 -2.399248 -0.663199
1 -2.140268 -1.215943 1.437451
35 0.506219 0.000021 -0.192545
cf3br_dmf

6 -2.820557 0.236737 -0.000805
9 -3.366654 0.090083 1.198805
9 -3.545683 -0.448609 -0.873897
9 -2.881364 1.521593 -0.329036
6 2.430285 0.095752 0.002287
8 1.833010 -0.962645 0.002236
7 3.769499 0.238497 -0.000161
1 1.902753 1.067038 0.004379
6 4.630564 -0.917151 -0.003291
1 4.010292 -1.811341 -0.003333
1 5.268665 -0.917587 -0.892435
1 5.271978 -0.919979 0.883461
6 4.390940 1.535287 0.000140
1 5.020759 1.666918 0.886048
1 5.017163 1.669074 -0.887990
1 3.624936 2.311711 0.002634
35 -0.994606 -0.377300 0.001075

cf3br_dmso

6 2.485049 0.217213 0.002835
9 2.503057 1.543291 -0.065133
9 3.159657 -0.260043 -1.033186
9 3.110478 -0.149159 1.112448
35 0.669037 -0.435493 -0.005232
16 -3.163720 -0.233427 -0.004522
8 -2.084133 -1.256580 -0.020455
6 -2.799496 0.925948 -1.329390
1 -2.911856 0.378949 -2.265455
1 -3.509407 1.754310 -1.296844
1 -1.772796 1.281139 -1.226545
6 -2.800636 0.882169 1.357679
1 -3.508615 1.712775 1.349995
1 -2.916390 0.305724 2.275484
1 -1.772890 1.238054 1.268549

cf3br_methanol

6 1.705669 0.110656 -0.022026
9 1.943262 1.339760 -0.457284
9 2.296954 -0.744632 -0.843365
9 2.248584 -0.019414 1.179110
6 -3.685474 0.727018 -0.017010
1 -3.388299 1.242003 0.896701
1 -3.318506 1.306383 -0.872412
1 -4.780398 0.693209 -0.052661
8 -3.117841 -0.566454 0.035745
1 -3.364861 -1.044418 -0.759037
35 -0.192159 -0.224943 0.052272

cf3br_water

6 -1.341124 0.000091 0.021920
9 -1.825620 1.127385 -0.477909
9 -1.758715 -0.114277 1.274789
9 -1.833690 -1.012543 -0.675991
35 0.584896 -0.000243 -0.051711

8 3.564486 0.000177 -0.034520
1 3.910573 0.764186 0.432582
1 3.911159 -0.762741 0.433962
cf3i_acetone
6 2.483821 0.161040 -0.002178
9 3.070531 -0.360486 1.070506
9 2.716442 1.470749 0.000088
9 3.065517 -0.355816 -1.079842
6 -3.434787 0.044799 -0.001378
8 -2.523116 -0.751050 0.004323
6 -4.865830 -0.412941 -0.004639
1 -5.435860 0.098994 0.775085
1 -5.326830 -0.145339 -0.960442
1 -4.918115 -1.490970 0.134085
6 -3.201486 1.528725 -0.000978
1 -3.821371 2.018516 -0.755919
1 -3.504026 1.935144 0.969273
1 -2.150290 1.754418 -0.170510
53 0.373183 -0.243059 0.002115
cf3i_acn
6 -2.288256 0.000734 0.000012
9 -2.765445 -1.238543 0.066988
9 -2.764197 0.562864 -1.107005
9 -2.764123 0.678872 1.040049
6 4.083667 -0.000163 -0.000031
7 2.935911 -0.001897 -0.000110
6 5.531888 0.002057 0.000072
1 5.903700 0.522662 0.883848
1 5.906169 -1.022729 0.008582
1 5.903868 0.507976 -0.892130
53 -0.143114 -0.000738 -0.000003
cf3i_diethylether
6 2.538084 0.000008 0.111105
9 2.949521 1.147632 0.638237
9 3.153209 -0.163215 -1.054155
9 2.916144 -0.984119 0.919126
53 0.402617 -0.000263 -0.144315
8 -2.611455 0.000213 -0.150909
6 -2.978965 -1.176441 0.539841
1 -4.047653 -1.128296 0.795171
6 -2.977973 1.177096 0.539976
1 -2.418580 1.244926 1.485419
1 -4.046519 1.129510 0.795959
6 -2.698717 2.370953 -0.336483
1 -2.994322 3.289545 0.174720
1 -1.636027 2.440302 -0.575809
1 -3.258036 2.297621 -1.270977
6 -2.699768 -2.370500 -0.336363
1 -2.996737 -3.288855 0.174483
1 -3.257964 -2.296673 -1.271486
1 -1.636871 -2.440718 -0.574491

1 -2.420183 -1.244500 1.485642
cf3i_dmf
6 -2.879145 0.266972 -0.000783
9 -3.364695 0.311902 1.237570
9 -3.604831 -0.608934 -0.690907
9 -3.058241 1.466499 -0.550671
53 -0.800442 -0.278722 0.000824
6 2.693390 0.222949 0.001549
8 2.007592 -0.784498 0.001500
7 4.035966 0.247723 -0.000236
1 2.247372 1.232867 0.003125
6 4.795000 -0.978477 -0.002611
1 4.101737 -1.817083 -0.002460
1 5.430489 -1.032133 -0.891631
1 5.433108 -1.033972 0.884414
6 4.768250 1.486559 -0.000055
1 5.406251 1.561235 0.886199
1 5.403594 1.563081 -0.888062
1 4.073331 2.326954 0.001857
cf3i_dmso
6 -2.582493 0.293641 -0.000483
9 -2.669778 1.578589 -0.341454
9 -3.131741 0.155098 1.203502
9 -3.311547 -0.406796 -0.864783
16 3.340772 -0.210645 0.000748
8 2.187049 -1.156370 0.002012
53 -0.532376 -0.365389 0.000626
6 3.059972 0.947887 1.343792
1 3.131864 0.379057 2.270736
1 3.829121 1.721809 1.323124
1 2.062269 1.379260 1.247277
6 3.061377 0.942476 -1.347230
1 3.830279 1.716721 -1.328697
1 3.134713 0.369933 -2.271747
1 2.063435 1.374074 -1.253798
cf3i_methanol
6 -1.900594 0.135344 0.023519
9 -2.235760 1.247802 -0.621469
9 -2.330073 0.241873 1.276827
9 -2.542042 -0.879343 -0.545673
53 0.226160 -0.171711 -0.034125
6 3.815993 0.750224 0.022600
1 3.480017 1.328572 -0.837843
1 3.577063 1.312753 0.931941
1 4.901555 0.623246 -0.047423
8 3.140024 -0.492931 -0.027967
1 3.413200 -1.026812 0.721780
cf3i_water
6 1.593606 -0.000251 0.025038
9 2.097000 -0.669680 -1.006009
9 2.035057 -0.571176 1.141056

9 2.068479 1.239937 -0.017762
8 -3.529733 -0.000554 -0.017569
1 -3.893209 -0.766745 0.433378
1 -3.894030 0.763022 0.437038
53 -0.553611 0.000338 -0.036522
se(cf3)2_acetone
6 3.441848 -0.489787 -0.002879
8 2.546340 -0.652870 -0.798016
6 4.882347 -0.487874 -0.433397
1 5.401247 0.388824 -0.036610
1 5.384386 -1.367031 -0.017749
1 4.952111 -0.509455 -1.519187
6 3.177769 -0.267790 1.460777
1 3.872683 -0.841124 2.078635
1 3.342624 0.789832 1.690027
1 2.148862 -0.524466 1.706994
34 -0.422799 -0.588372 -0.229500
6 -0.318929 1.378118 -0.068854
6 -2.367811 -0.665900 0.102157
9 0.959612 1.722047 0.058992
9 -0.978683 1.828824 0.994955
9 -0.806083 1.998543 -1.136987
9 -2.697592 -0.411101 1.364947
9 -3.062226 0.164562 -0.669399
9 -2.747118 -1.915047 -0.174932
se(cf3)2_acn
6 4.096906 -0.663419 0.005678
7 2.963019 -0.824348 -0.077858
6 5.527108 -0.457981 0.110736
1 5.899905 -0.891860 1.039809
1 6.035627 -0.931831 -0.730275
1 5.751647 0.609753 0.103809
34 -0.258366 -0.629019 -0.096369
6 -0.084806 1.336042 -0.011340
6 -2.224426 -0.627895 0.048922
9 1.145798 1.658086 -0.392301
9 -0.272696 1.807870 1.217796
9 -0.948582 1.952356 -0.813344
9 -2.833918 -0.184432 -1.046012
9 -2.669955 0.091667 1.074724
9 -2.590932 -1.897710 0.235162
se(cf3)2_diethylether
8 -2.571872 -0.069107 -0.571189
6 -3.326031 -1.052615 0.102120
1 -4.367276 -1.020330 -0.253176
6 -3.096772 1.228489 -0.391804
1 -3.030128 1.513938 0.669306
1 -4.163838 1.231150 -0.661399
6 -2.336185 2.201799 -1.256043
1 -2.756846 3.204091 -1.149566
1 -1.283556 2.240172 -0.972498

1 -2.398129 1.909410 -2.306143
6 -2.722345 -2.408473 -0.160178
1 -3.317080 -3.184949 0.325972
1 -2.694018 -2.614735 -1.232080
1 -1.703830 -2.465214 0.228443
1 -3.343891 -0.837729 1.180920
34 0.507427 -0.327338 -0.526055
6 0.273327 0.318457 1.328114
6 2.470277 -0.118265 -0.541934
9 0.125383 1.640222 1.380724
9 -0.824933 -0.232113 1.838329
9 1.300905 -0.005266 2.104427
9 2.861439 1.087394 -0.139918
9 2.851423 -0.284459 -1.809542
9 3.108832 -1.017979 0.197530
se(cf3)2_dmf
6 2.575131 -0.456778 0.060558
8 1.934534 -0.034893 -0.885650
7 3.914639 -0.439676 0.161322
1 2.085774 -0.902401 0.944102
6 4.724797 0.113149 -0.895503
1 4.068290 0.464346 -1.689020
1 5.321813 0.950035 -0.520755
1 5.403766 -0.646636 -1.294234
6 4.590846 -0.957336 1.320976
1 5.266013 -1.774003 1.046238
1 5.179813 -0.174865 1.809977
1 3.860062 -1.337600 2.035536
34 -0.820152 -0.481785 -0.511242
6 -0.572160 1.361625 0.171752
6 -2.676251 -0.704274 0.125506
9 -1.727906 1.915039 0.528653
9 -0.019092 2.124359 -0.758781
9 0.227320 1.377724 1.240112
9 -3.558475 0.083963 -0.480551
9 -3.000796 -1.971445 -0.155572
9 -2.813639 -0.527378 1.437987
se(cf3)2_dmso
16 3.270760 -0.754085 -0.291429
8 2.007412 -0.553530 -1.054914
34 -0.722521 -0.558096 -0.444450
6 -2.603397 -0.477651 0.154527
6 -0.266383 1.306785 0.033596
9 -1.343926 2.025872 0.328784
9 0.368350 1.903880 -0.963857
9 0.542703 1.347087 1.102619
9 -3.367132 0.346165 -0.555918
9 -3.079250 -1.717263 -0.006537
9 -2.741927 -0.148862 1.437446
6 3.850999 0.877470 0.185807
1 4.734266 0.776307 0.818959

1 4.114380 1.397090 -0.735404
1 3.053342 1.412220 0.702039
6 2.806333 -1.311418 1.351864
1 2.364772 -2.301315 1.237188
1 3.698781 -1.374813 1.976893
1 2.074024 -0.623679 1.776217
se(cf3)2_methanol
6 -1.893542 -0.553100 0.017094
9 -2.277029 -1.831739 0.079339
9 -2.470516 -0.005595 -1.047104
9 -2.356303 0.071747 1.094910
6 3.501724 -1.616088 0.107576
1 3.078116 -2.084389 0.996267
1 3.258047 -2.238442 -0.761372
1 4.590085 -1.576063 0.224183
8 2.936232 -0.324115 0.014310
1 3.278735 0.117014 -0.766588
34 0.077653 -0.597701 -0.076733
6 0.358894 1.360846 0.017726
9 -0.766234 2.031658 -0.202537
9 1.244087 1.733048 -0.908042
9 0.832938 1.728289 1.199833
se(cf3)2_water
6 -1.780266 -0.081916 0.000275
9 -2.063155 0.648816 -1.072790
9 -2.061767 0.648903 1.073659
9 -2.586208 -1.146875 0.000815
8 2.875570 -1.554106 0.000563
1 3.323554 -1.177191 -0.761225
1 3.321371 -1.182096 0.766019
34 0.052904 -0.815671 -0.000802
6 1.000136 0.922240 -0.000061
9 0.166138 1.952638 -0.001445
9 1.784146 1.031037 1.074019
9 1.786687 1.030257 -1.072404
te(cf3)2_acetone
6 3.392270 -0.454747 0.128993
8 2.472732 -0.850735 -0.553657
6 4.816498 -0.679672 -0.285629
1 5.382639 0.253689 -0.226653
1 5.286543 -1.378170 0.413682
1 4.860203 -1.087723 -1.293330
6 3.168559 0.294313 1.409845
1 3.926006 0.047542 2.155971
1 3.255932 1.365247 1.198849
1 2.169883 0.103237 1.800065
6 -0.001751 1.432773 -0.219770
6 -2.503817 -0.346849 0.214741
9 1.113408 1.696884 -0.902225
9 0.154952 1.944394 1.005828
9 -1.002768 2.091421 -0.798718

9 -2.706884 0.499782 1.226617
9 -3.174282 0.125146 -0.836178
9 -3.057907 -1.522423 0.547721
52 -0.381390 -0.720956 -0.178766
te(cf3)2_acn
6 3.509691 -0.794422 0.007745
7 2.605047 -1.501834 -0.020141
6 4.626685 0.123840 0.038991
1 5.302051 -0.132215 0.856609
1 5.172916 0.081703 -0.904388
1 4.251588 1.138034 0.189276
6 0.619624 1.148593 -0.012662
6 -2.353278 0.061874 0.013162
9 1.401078 1.308811 -1.086133
9 1.403024 1.313910 1.059706
9 -0.273633 2.133361 -0.013635
9 -2.626363 0.805293 -1.058004
9 -2.602702 0.806715 1.089204
9 -3.212766 -0.967868 0.023214
52 -0.349538 -0.815692 -0.007944
te(cf3)2_diethylether
8 -2.540538 -0.508585 0.044370
6 -3.262479 0.019126 1.142785
1 -4.288910 -0.373645 1.111809
6 -3.210814 -0.282686 -1.183088
1 -3.252654 0.796422 -1.387472
1 -4.246622 -0.639536 -1.090242
6 -2.508046 -1.012328 -2.298151
1 -3.065424 -0.885694 -3.228841
1 -1.498788 -0.628833 -2.451618
1 -2.442747 -2.079670 -2.077774
6 -2.594872 -0.372072 2.435294
1 -3.188289 -0.013746 3.279209
1 -2.508993 -1.457862 2.510926
1 -1.596878 0.060523 2.514734
1 -3.326174 1.112367 1.051817
6 0.003431 1.478554 -0.181872
6 2.602513 -0.321791 0.029309
9 -0.621617 1.694138 -1.342153
9 -0.792317 1.947830 0.782391
9 1.115649 2.207978 -0.179696
9 3.016839 0.211299 -1.119262
9 3.169037 -1.532598 0.144054
9 3.075227 0.438919 1.015324
52 0.440308 -0.645819 0.116172
te(cf3)2_dmf
6 2.712082 -0.462746 0.300516
8 1.971877 -0.521086 -0.671431
7 4.042424 -0.331995 0.244630
1 2.323444 -0.512627 1.330284
6 4.722943 -0.233892 -1.024091

1 3.984871 -0.285255 -1.821633
1 5.264862 0.713887 -1.090508
1 5.438761 -1.053359 -1.135977
6 4.844055 -0.265236 1.439189
1 5.572779 -1.081148 1.462614
1 5.386857 0.683588 1.487696
1 4.204661 -0.344402 2.318712
6 -0.252321 1.441062 -0.085900
6 -2.836166 -0.343042 0.262376
9 -1.343437 2.167209 0.152007
9 0.311482 1.905844 -1.198108
9 0.607240 1.675179 0.916627
9 -3.502955 0.410262 -0.613879
9 -3.421216 -1.554159 0.275237
9 -3.019704 0.199610 1.468643
52 -0.732201 -0.686162 -0.254797

te(cf3)2_dmso

16 3.361050 -0.766185 -0.177014
8 2.037905 -0.752090 -0.874258
6 -2.711151 -0.243444 0.222194
6 -0.048296 1.416352 -0.017512
9 -1.105101 2.194587 0.200272
9 0.606470 1.903173 -1.069756
9 0.769967 1.559029 1.043702
9 -3.340638 0.579030 -0.618302
9 -3.354549 -1.423538 0.184470
9 -2.865598 0.255311 1.451615
52 -0.626997 -0.668996 -0.314667
6 3.921781 0.935783 -0.102280
1 4.858569 0.976475 0.456347
1 4.090838 1.253478 -1.131022
1 3.156426 1.557484 0.361522
6 3.027552 -0.979490 1.572513
1 2.610486 -1.978838 1.696581
1 3.964929 -0.899261 2.125590
1 2.308263 -0.229420 1.902487

te(cf3)2_water

6 -1.915719 0.113891 0.000089
9 -2.152171 0.866140 -1.073806
9 -2.151718 0.866463 1.073866
9 -2.809109 -0.886886 0.000415
8 2.889137 -1.382395 0.000172
1 3.313244 -0.981025 -0.763704
1 3.312702 -0.983322 0.765540
52 0.060324 -0.828034 -0.000146
6 1.093226 1.099098 -0.000023
9 0.241824 2.117786 -0.000584
9 1.883769 1.229337 -1.073489
9 1.882858 1.229754 1.074040

dcm

6 -0.000000 -0.000000 0.759090

```
1   -0.896963    0.000000    1.372342
17   0.000000    1.470398   -0.214683
17  -0.000000   -1.470398   -0.214683
1    0.896963   -0.000000    1.372342
tcm
17  -0.000000    1.677584   -0.083387
6   -0.000000   -0.000000    0.452482
1   -0.000000   -0.000000    1.537850
17  -1.452830   -0.838792   -0.083387
17   1.452830   -0.838792   -0.083387
cf3br_dcm
6   -1.886492    0.492270    0.163166
9   -1.910606    1.287180   -0.888758
9   -1.277845    1.119374    1.158577
9   -3.128389    0.227790    0.528199
35  -0.948721   -1.145039   -0.253035
6    2.301068    0.457317    0.755321
1    1.380784    0.226799    1.284462
17   2.968869   -1.053527    0.136233
17   1.922323    1.614412   -0.520634
1    3.038288    0.907904    1.413522
cf3br_tcm
6     2.199344   -0.717643   -0.129570
9     3.366875   -0.824828   -0.735556
9     1.307482   -1.435900   -0.795477
9     2.304919   -1.198078    1.093648
6    -1.934411   -0.084540   -0.136513
1    -1.050983   -0.108576   -0.766435
17   -2.351551    1.605556    0.130827
17   -3.224313   -0.933159   -0.981160
17   -1.530179   -0.885435    1.378708
35    1.641447    1.133502   -0.076656
cf3I_dcm
6    -2.552261    0.378225    0.149150
9    -3.084380    0.805640   -0.985875
9    -2.464726    1.403957    0.984053
9    -3.364025   -0.524810    0.679191
6     3.051237    0.279673    0.844298
1     2.160996    0.423243    1.450858
17    2.925965   -1.302671    0.063602
17    3.152693    1.602921   -0.311751
1     3.952845    0.280886    1.449957
53   -0.608051   -0.470167   -0.202628
cf3I_tcm
6    -2.890595    0.633760   -0.206995
9    -3.762990    0.073110   -1.029304
9    -2.485427    1.777576   -0.737922
9    -3.497643    0.892894    0.939905
6     2.542838    0.265708   -0.162385
1     1.632887    0.584079   -0.662606
17    2.475679   -1.493475   -0.017107
```

17	3.911387	0.764721	-1.146498
53	-1.212056	-0.674414	0.111859
17	2.578061	1.027040	1.422208
Se(cf3)2_dcm			
34	-0.609712	-0.465541	-0.605246
6	-0.559739	1.482226	-0.279205
6	-2.283485	-0.804721	0.380942
9	-1.635173	2.096815	-0.757387
9	0.510896	1.947179	-0.911639
9	-0.459553	1.782951	1.007590
9	-2.206745	-0.454740	1.658646
9	-3.329271	-0.183967	-0.148025
9	-2.496127	-2.118713	0.315792
17	3.041808	-0.814817	-1.191372
6	2.953155	-1.063938	0.555302
1	3.842546	-1.606404	0.862687
17	2.883198	0.447296	1.457349
1	2.046756	-1.624468	0.767038
Se(cf3)2_tcm			
34	-0.829905	-0.304863	-0.561645
6	-1.160297	1.545553	0.036394
6	-2.512913	-1.051471	0.143510
9	-2.336060	2.008981	-0.370507
9	-0.200764	2.299426	-0.492514
9	-1.111013	1.672335	1.356819
9	-2.677165	-0.809891	1.438362
9	-3.586634	-0.599190	-0.491888
9	-2.445278	-2.369513	-0.037267
17	2.754164	0.488374	-1.433225
6	3.231365	-0.167758	0.133230
1	4.307163	-0.053509	0.220031
17	2.486676	0.729019	1.450677
17	2.863449	-1.885536	0.239610
Te(cf3)2_dcm			
6	-0.337226	1.562561	-0.420179
6	-2.489380	-0.529829	0.536910
9	-1.372149	2.159631	-1.005856
9	0.766068	1.879924	-1.094535
9	-0.232283	2.054471	0.809268
9	-2.449013	0.103612	1.705728
9	-3.417713	0.060687	-0.208935
9	-2.877679	-1.789730	0.759503
17	3.109721	-1.001661	-1.010398
6	3.198414	-0.968169	0.756394
1	4.150283	-1.401383	1.049765
17	3.098109	0.661680	1.411003
1	2.359454	-1.541068	1.142383
52	-0.539015	-0.613127	-0.440918
Te(cf3)2_tcm			
6	1.423476	1.718212	0.034996
6	2.605421	-1.193519	0.127656

```
9     1.821260    1.965973    1.279396
9     0.447025    2.578861   -0.264277
9     2.452430    1.961972   -0.771804
9     3.480971   -0.893431   -0.827180
9     3.139430   -0.829795    1.290469
9     2.446404   -2.520689    0.139075
17   -2.744815    1.433829   -0.429310
6    -3.576754   -0.057483    0.011715
1    -4.643550    0.126923   -0.066185
17   -3.174818   -1.358100   -1.107114
52    0.640040   -0.304987   -0.209585
17   -3.223842   -0.513193    1.672149
```