

## Supplementary Information for

### A recyclable and base-free method for the synthesis of 3-iodothiophenes by the iodoheterocyclization of 1-mercapto-3-yn-2-ols in ionic liquids

Raffaella Mancuso,<sup>\*,a</sup> Christian S. Pomelli,<sup>b</sup> Cinzia Chiappe,<sup>b</sup> Richard C. Larock<sup>c</sup> and Bartolo Gabriele<sup>a,\*</sup>

*raffaella.mancuso@unical.it; bartolo.gabriele@unical.it*

<sup>a</sup> Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Via P. Bucci, 12/C,  
87036 Arcavacata di Rende (CS), Italy

<sup>b</sup> Dipartimento di Farmacia, Università di Pisa, Via Bonanno 33, 56126 Pisa, Italy

<sup>c</sup> Department of Chemistry, Iowa State University, Ames, Iowa 50011, United States

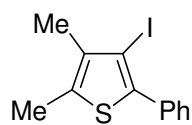
## Table of Contents

**Pages S2–S6**      **Copy of <sup>1</sup>H NMR Spectra for Products 2a-2j**

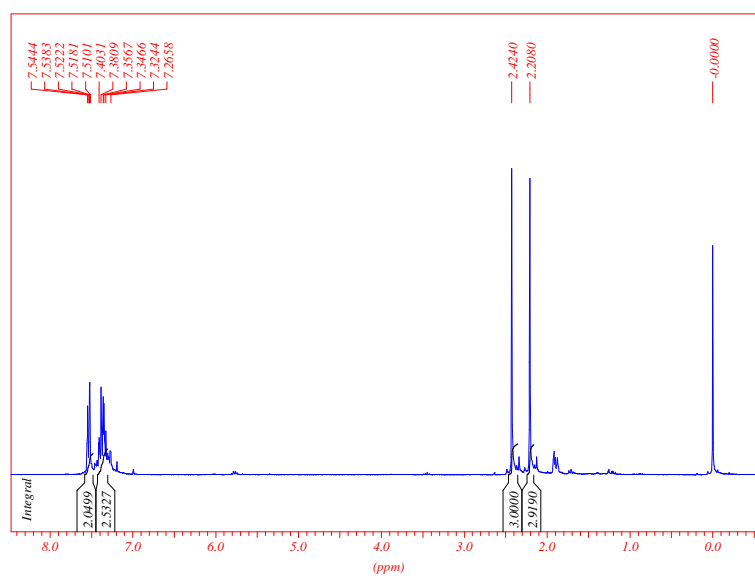
**Pages S7–S97**      **Tables of Atom Coordinates and Absolute Energies**

S 2

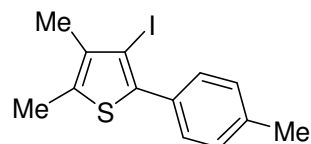
3-Iodo-4,5-dimethyl-2-phenylthiophene (**2a**)



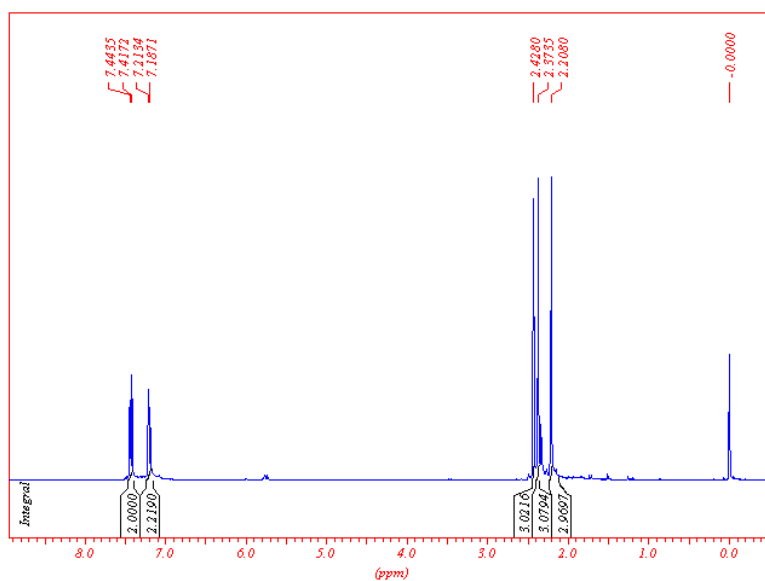
$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )



3-Iodo-4,5-dimethyl-2-*p*-tolylthiophene (**2b**)

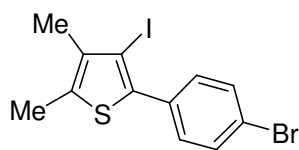


$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )

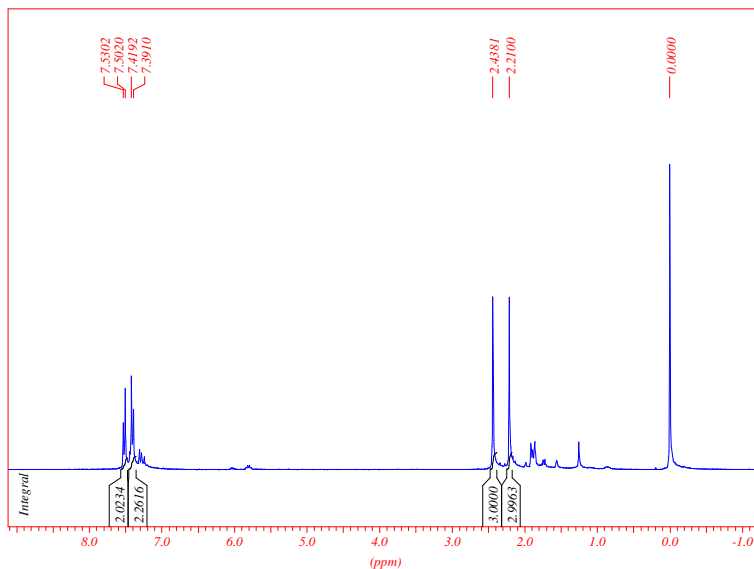


S 3

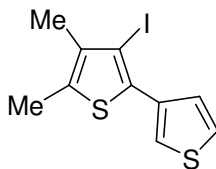
2-(4-Bromophenyl)-3-iodo-4,5-dimethylthiophene (**2c**)



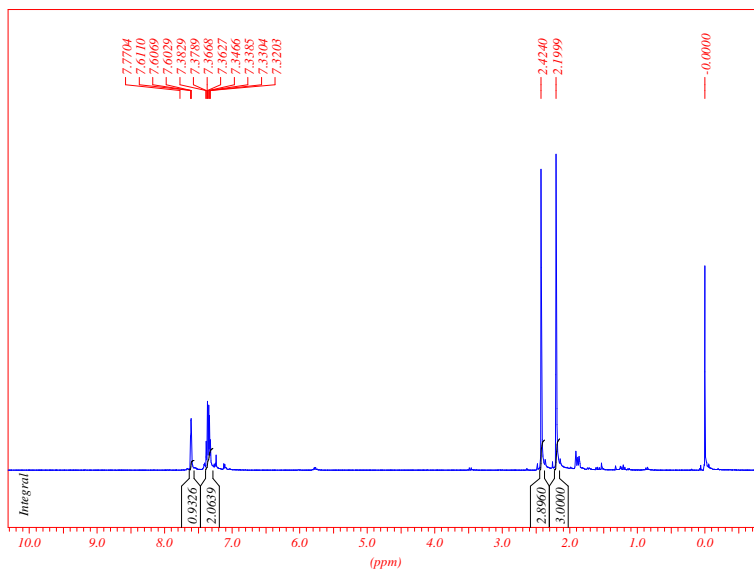
$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )



3-(3-Iodo-4,5-dimethylthiophen-2-yl)thiophene (**2d**)

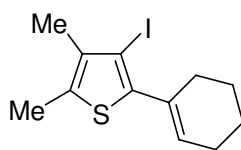


$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )

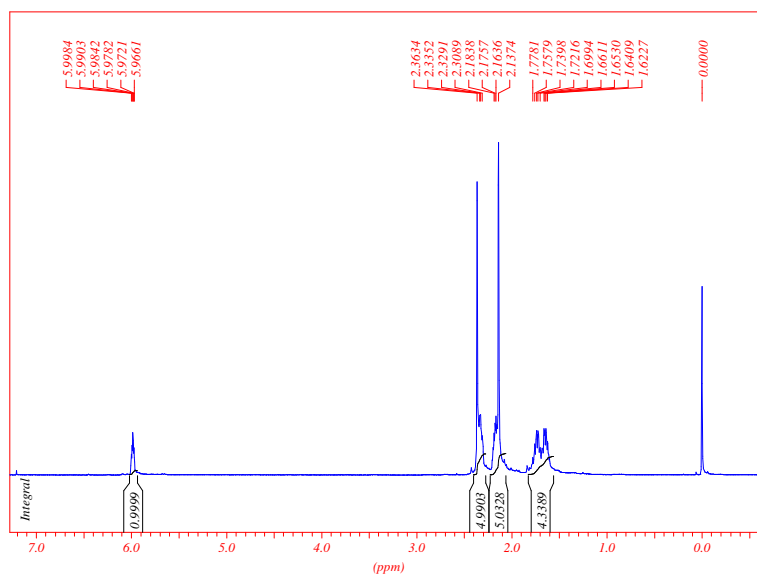


S 4

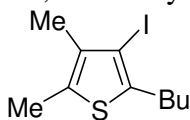
2-Cyclohex-1-enyl-3-iodo-4,5-dimethylthiophene (**2e**)



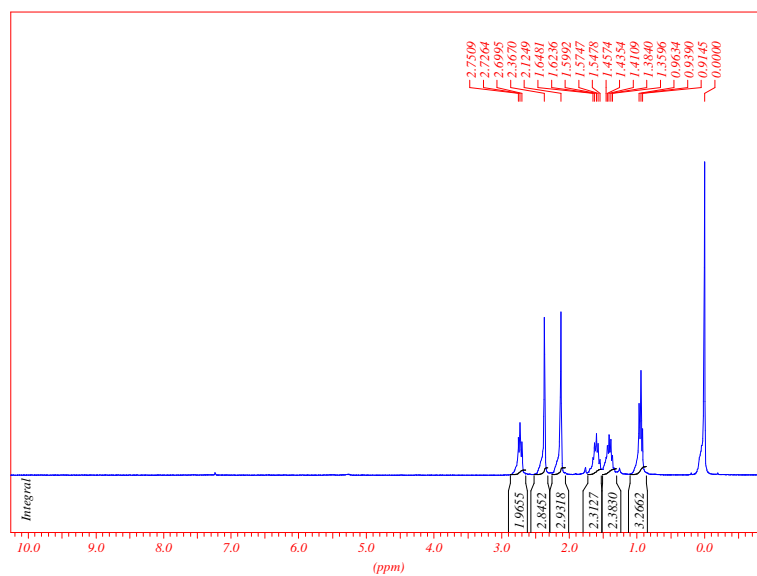
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



2-Butyl-3-iodo-4,5-dimethylthiophene (**2f**)

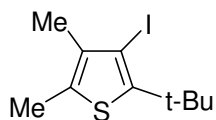


$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )

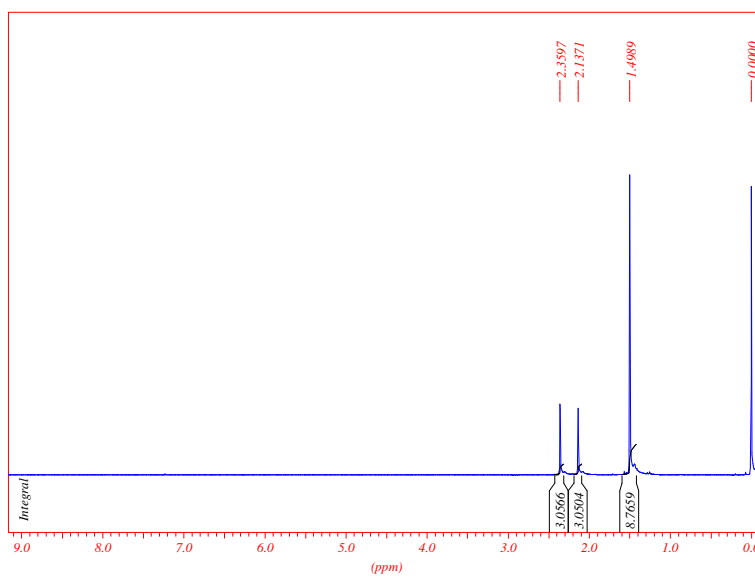


S 5

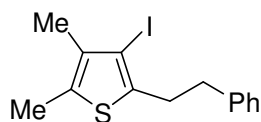
2-*tert*-Butyl-3-iodo-4,5-dimethylthiophene (**2g**)



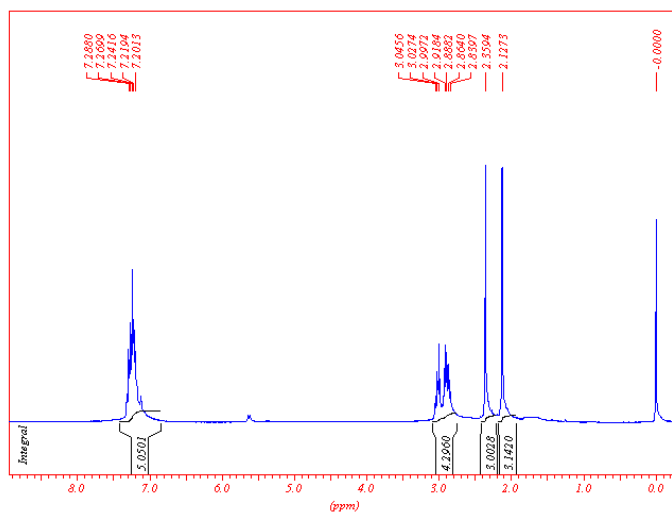
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



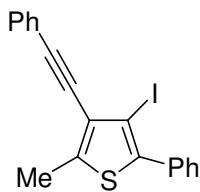
3-Iodo-4,5-dimethyl-2-phenethylthiophene (**2h**)



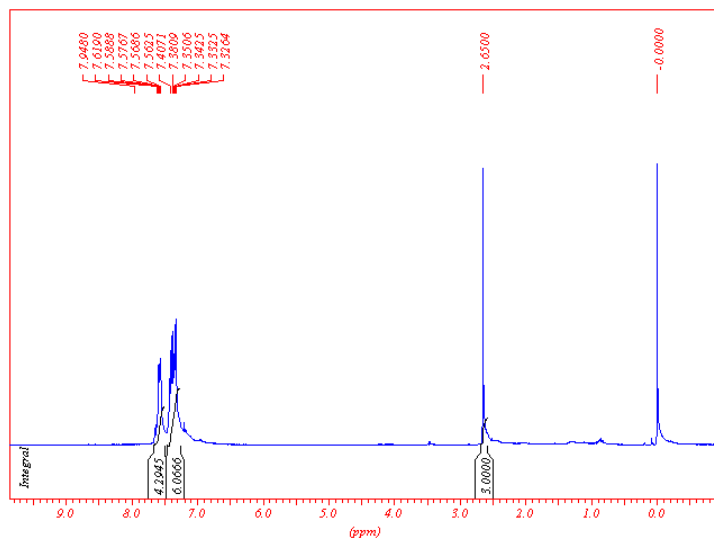
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



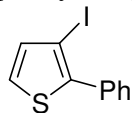
3-Iodo-5-methyl-2-phenyl-4-phenylethynylthiophene (**2i**)



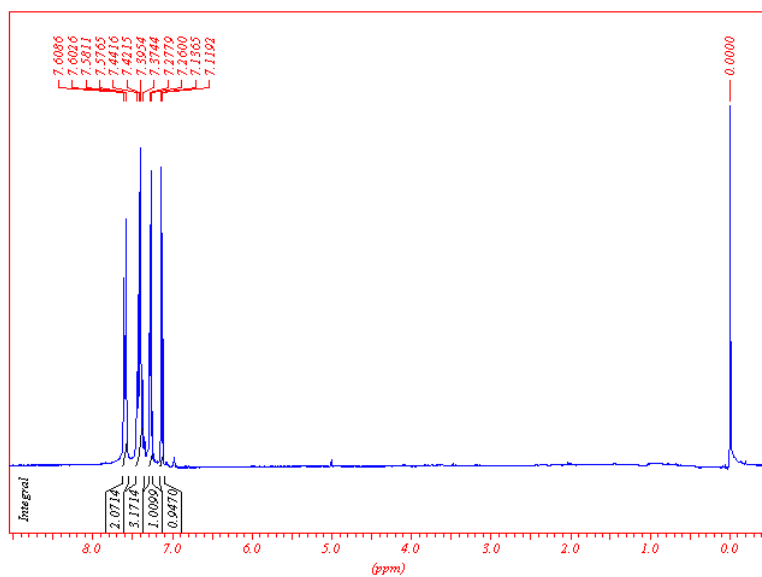
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



3-Iodo-2-phenylthiophene (**2j**)



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



**Tables of Atom Coordinates and Absolute Energies**

R(S-C)	Bu-Br	Ph-Br	Bu-NO3	Ph-NO3	Bu-EtSO4	Ph-EtSO4
5.4	-903.2908326	-977.0982731	-1437.671004	-1511.480178	-2433.678195	-2507.486748
5.2	-903.2937253	-977.1012715	-1437.671085	-1511.479323	-2433.682331	-2507.490936
5.0	-903.2933394	-977.1015947	-1437.660065	-1511.469575	-2433.683567	-2507.492579
4.8	-903.2907438	-977.0997702	-1437.658629	-1511.468468	-2433.682671	-2507.492101
4.6	-903.2773686	-977.0942037	-1437.641208	-1511.466252	-2433.674457	-2507.490531
4.4	-903.2805807	-977.0956611	-1437.647523	-1511.465023	-2433.676422	-2507.487082
4.2	-903.2833401	-977.0966631	-1437.641177	-1511.451029	-2433.676101	-2507.484901
4.0	-903.2856461	-977.0971393	-1437.646942	-1511.45615	-2433.678498	-2507.484602
3.8	-903.2873927	-977.0983582	-1437.654755	-1511.463275	-2433.679951	-2507.487528
3.6	-903.2882612	-977.0996805	-1437.665573	-1511.474335	-2433.678991	-2507.490186
3.4	-903.2881128	-977.1002298	-1437.679751	-1511.459231	-2433.681475	-2507.492645
3.2	-903.2868302	-977.1003013	-1437.652527	-1511.464598	-2433.682858	-2507.495056
3.0	-903.2868735	-977.1004762	-1437.659154	-1511.470945	-2433.674503	-2507.487365
2.8	-903.2883474	-977.1011407	-1437.667631	-1511.478591	-2433.683368	-2507.495522
2.6	-903.2919794	-977.1030228	-1437.678455	-1511.48815	-2433.695035	-2507.505899
2.4	-903.2987627	-977.1072047	-1437.691904	-1511.500567	-2433.709408	-2507.516834
2.2	-903.3118778	-977.1200185	-1437.707532	-1511.515586	-2433.725885	-2507.532781
2.0	-903.3255051	-977.1332668	-1437.722518	-1511.530286	-2433.741813	-2507.547423
1.8	-903.3320019	-977.139171	-1437.729417	-1511.536842	-2433.749516	-2507.554326
1ec	-903.0352160	-976.8748132	-1437.383262	-1511.213087	-2433.258297	-2507.09883
1r	-903.0728651	-976.9125580	-1437.436389	-1511.276072	-2433.318109	-2507.15822
1ts		-976.8673624				

Absolute energies in Hartrees. Zero point energy enclosed.

Molecular geometries in xyz format

33  
Bu-Br 1ec  
6 -0.682422 1.750045 0.717552  
6 0.356812 1.124234 0.632959  
6 1.713791 0.523685 0.600162  
6 2.698016 1.759212 0.765097  
6 1.844716 -0.499072 1.743427  
1 1.054769 -1.246020 1.650232  
1 2.811589 -0.996014 1.670614  
1 1.773183 -0.013587 2.720231  
6 2.767074 2.594670 -0.515877  
1 3.347508 3.501818 -0.335150  
1 1.764757 2.876507 -0.855259  
8 1.838703 -0.095321 -0.662340  
1 2.712296 -0.554211 -0.742955  
53 -1.912179 -0.853629 0.233481  
1 2.297313 2.371164 1.578570  
1 3.245445 2.028223 -1.315186  
16 4.388048 1.340316 1.387178  
35 -3.665445 -2.781216 -0.057947  
1 4.710284 0.404650 0.427069  
35 4.812945 -1.441332 -1.093501  
6 -1.813434 2.675781 0.809913  
6 -2.372209 3.107991 -0.559537  
1 -1.476557 3.561498 1.363815  
1 -2.612144 2.222820 1.407337  
6 -3.542363 4.088144 -0.432060  
1 -1.566120 3.562453 -1.145164  
1 -2.691812 2.217099 -1.108782  
6 -4.104079 4.525973 -1.787980  
1 -4.340190 3.623545 0.160262  
1 -3.218003 4.972196 0.131448  
1 -4.937989 5.223883 -1.668261  
1 -3.337521 5.022443 -2.391206  
1 -4.467613 3.666565 -2.359493

33  
Bu-Br 1r  
6 -0.775142 0.195435 1.119436  
6 0.076600 -0.671264 0.567176  
6 -0.493078 -2.041860 0.209787  
6 -1.717765 -2.236834 1.146548  
6 -0.838661 -2.094077 -1.286042  
1 0.055686 -1.870923 -1.871145  
1 -1.186534 -3.093297 -1.557729  
1 -1.608169 -1.362629 -1.545519  
6 -2.773181 -3.245192 0.712719  
1 -3.542985 -3.355854 1.481393  
1 -2.299537 -4.220409 0.569546  
8 0.393439 -3.120665 0.531333  
1 1.294857 -2.831199 0.324599  
53 2.150168 -0.245252 0.063329  
1 -1.300777 -2.533528 2.110958  
1 -3.263593 -2.956788 -0.218603  
16 -2.409230 -0.540347 1.429329  
35 5.146559 0.299607 -0.672841  
1 -3.735086 -0.138821 -0.225978  
35 -4.777156 0.151762 -1.261939  
6 -0.577999 1.632538 1.499011  
6 -1.220577 2.629920 0.516555  
1 0.497872 1.820821 1.551158  
1 -0.984606 1.800944 2.504236  
6 -0.996434 4.089758 0.924970  
1 -0.801747 2.458529 -0.481075  
1 -2.297030 2.435573 0.437763  
6 -1.622728 5.089569 -0.051875  
1 -1.408742 4.252351 1.929043  
1 0.080525 4.279761 1.001999



## S9

1	-1.447326	6.122137	0.265300
1	-1.201968	4.974137	-1.055522
1	-2.704904	4.942559	-0.129188

33

Bu-Br RCS=1.8

6	-0.900356	0.769597	0.295910
6	-0.117215	-0.287010	0.527913
6	-0.786439	-1.482991	1.201083
6	-2.011720	-0.898301	1.958159
6	-1.149772	-2.540719	0.148212
1	-0.247590	-2.839645	-0.389174
1	-1.570956	-3.425261	0.631560
1	-1.866986	-2.152077	-0.579278
6	-3.153049	-1.852494	2.283222
1	-3.920531	-1.350560	2.878880
1	-2.765334	-2.688548	2.871922
8	0.023988	-2.083713	2.219137
1	0.941335	-2.073497	1.907284
53	1.973255	-0.443725	-0.044303
1	-1.608492	-0.479433	2.882256
1	-3.627929	-2.250672	1.384808
16	-2.558155	0.570888	0.968379
35	5.003640	-0.713338	-0.813449
1	-3.838800	-0.153521	-0.622026
35	-4.825573	-0.555156	-1.672169
6	-0.584949	2.061849	-0.400687
6	-0.263586	3.217156	0.566055
1	-1.429263	2.348050	-1.040734
1	0.270120	1.893293	-1.060881
6	0.038947	4.532225	-0.159736
1	-1.104300	3.362473	1.254789
1	0.597522	2.928832	1.178506
6	0.372170	5.682118	0.795752
1	0.876745	4.377543	-0.849593
1	-0.822219	4.810661	-0.780564
1	0.583844	6.607234	0.250906
1	-0.459009	5.881081	1.480552
1	1.251386	5.445640	1.403004

33

Bu-Br RCS=2.0

6	-0.825595	0.805409	0.248045
6	-0.072484	-0.247628	0.514549
6	-0.728293	-1.453685	1.182418
6	-1.960639	-0.910451	1.962457
6	-1.076876	-2.505376	0.118292
1	-0.173496	-2.778149	-0.431040
1	-1.472488	-3.404602	0.595438
1	-1.809686	-2.124154	-0.596611
6	-3.021152	-1.936416	2.347031
1	-3.787744	-1.481094	2.979722
1	-2.551106	-2.743870	2.915214
8	0.098926	-2.050088	2.189244
1	1.010999	-2.046380	1.862362
53	2.046438	-0.387620	-0.040749
1	-1.549776	-0.457249	2.866512
1	-3.515034	-2.365985	1.473499
16	-2.657595	0.498660	0.989448
35	5.045774	-0.648690	-0.767325
1	-3.822668	-0.308842	-0.587440
35	-4.767729	-0.774181	-1.663404
6	-0.596850	2.105438	-0.442062
6	-0.513369	3.312171	0.510552
1	-1.394810	2.273035	-1.176130
1	0.337622	2.018195	-1.005701
6	-0.285769	4.635106	-0.228197
1	-1.434006	3.373364	1.101934
1	0.303114	3.141531	1.220750
6	-0.191484	5.839385	0.713613
1	0.633277	4.563687	-0.821706

## S10

1	-1.101273	4.794878	-0.944889
1	-0.029504	6.769262	0.159981
1	-1.109020	5.955692	1.299875
1	0.638031	5.723407	1.418185

33

Bu-Br RCS=2.2

6	-0.751338	0.847686	0.194588
6	-0.042844	-0.209774	0.490341
6	-0.692748	-1.427935	1.140680
6	-1.932816	-0.924121	1.939786
6	-1.026580	-2.462834	0.055480
1	-0.120248	-2.713160	-0.499928
1	-1.408324	-3.375941	0.516661
1	-1.766128	-2.078431	-0.649859
6	-2.916467	-2.012609	2.364397
1	-3.678695	-1.601781	3.031322
1	-2.377953	-2.795443	2.905593
8	0.144083	-2.030188	2.135719
1	1.050768	-2.041403	1.795157
53	2.113688	-0.337524	-0.045401
1	-1.519431	-0.448037	2.830801
1	-3.424454	-2.463119	1.509617
16	-2.755710	0.434493	1.001907
35	5.070246	-0.605364	-0.713888
1	-3.813945	-0.409254	-0.519147
35	-4.731695	-0.931225	-1.624504
6	-0.606830	2.156121	-0.479857
6	-0.680586	3.367897	0.465513
1	-1.371709	2.247753	-1.260237
1	0.363680	2.143255	-0.990302
6	-0.526664	4.702010	-0.272015
1	-1.635374	3.348024	1.001970
1	0.104975	3.271485	1.222983
6	-0.593798	5.913817	0.662364
1	0.427936	4.710076	-0.811482
1	-1.310113	4.786033	-1.035631
1	-0.482091	6.851907	0.110245
1	-1.550733	5.950881	1.193105
1	0.199805	5.874626	1.415195

33

Bu-Br RCS=2.4

6	-0.676152	0.904201	0.113863
6	-0.040963	-0.167797	0.443195
6	-0.695724	-1.397550	1.061714
6	-1.951782	-0.929327	1.865029
6	-1.005946	-2.408667	-0.052005
1	-0.090815	-2.639908	-0.601720
1	-1.385027	-3.333885	0.385838
1	-1.742642	-2.017257	-0.755691
6	-2.879515	-2.068154	2.292648
1	-3.638664	-1.698827	2.986076
1	-2.296272	-2.839729	2.802520
8	0.135565	-2.009348	2.054868
1	1.035711	-2.061005	1.702503
53	2.175417	-0.293347	-0.053030
1	-1.547000	-0.447000	2.756679
1	-3.393475	-2.517631	1.441281
16	-2.858925	0.405383	0.977972
35	5.069300	-0.595815	-0.619215
1	-3.734797	-0.421103	-0.355398
35	-4.659096	-1.069515	-1.533422
6	-0.613785	2.218530	-0.539577
6	-0.790007	3.416495	0.408932
1	-1.362275	2.258092	-1.339095
1	0.368732	2.270606	-1.027947
6	-0.706228	4.760910	-0.320932
1	-1.755090	3.327303	0.918044
1	-0.020119	3.367947	1.186672
6	-0.880589	5.960530	0.615193

## S11

1	0.259753	4.836629	-0.834609
1	-1.472983	4.795335	-1.104805
1	-0.818269	6.906449	0.068879
1	-1.851755	5.929686	1.119430
1	-0.106841	5.971870	1.389364

33

Bu-Br RCS=2.6

6	-0.590268	0.966442	0.065159
6	-0.073201	-0.126676	0.435843
6	-0.717837	-1.360988	1.039878
6	-1.975470	-0.915913	1.864466
6	-1.030285	-2.353096	-0.088956
1	-0.121163	-2.561481	-0.658355
1	-1.388300	-3.289897	0.341144
1	-1.791604	-1.965881	-0.769611
6	-2.879791	-2.083884	2.268839
1	-3.616815	-1.750496	3.002342
1	-2.274828	-2.873756	2.721675
8	0.121275	-1.971537	2.025592
1	0.990166	-2.124338	1.629957
53	2.236401	-0.256025	-0.067377
1	-1.565567	-0.449396	2.762423
1	-3.419240	-2.489269	1.411310
16	-2.930048	0.438261	1.068381
35	5.016542	-0.627813	-0.556496
1	-3.570978	-0.287966	-0.027197
35	-4.578774	-1.201191	-1.524708
6	-0.640450	2.269015	-0.590670
6	-0.816468	3.469090	0.355492
1	-1.437695	2.251905	-1.342053
1	0.303537	2.363764	-1.146083
6	-0.843356	4.804351	-0.395023
1	-1.744923	3.339399	0.919968
1	-0.000416	3.468886	1.086107
6	-1.021213	6.007241	0.535971
1	0.085345	4.919744	-0.967064
1	-1.656383	4.788741	-1.130908
1	-1.039497	6.946304	-0.024829
1	-1.957952	5.936027	1.097594
1	-0.204220	6.068792	1.261889

33

Bu-Br RCS=2.8

6	-0.491905	1.022119	0.009753
6	-0.115210	-0.086731	0.439407
6	-0.762079	-1.307790	1.050779
6	-2.004479	-0.846477	1.893662
6	-1.101745	-2.295184	-0.073905
1	-0.204433	-2.513766	-0.658718
1	-1.463678	-3.227316	0.362574
1	-1.872194	-1.901160	-0.740891
6	-2.882874	-2.021230	2.337778
1	-3.599283	-1.683417	3.089177
1	-2.260526	-2.804630	2.778372
8	0.086436	-1.924089	2.026209
1	0.927390	-2.139944	1.602652
53	2.281969	-0.255909	-0.082085
1	-1.573499	-0.366883	2.775101
1	-3.447104	-2.435155	1.500271
16	-3.005444	0.489095	1.122410
35	4.985567	-0.731776	-0.532212
1	-3.629959	-0.245047	0.070748
35	-4.630216	-1.247980	-1.528067
6	-0.579523	2.316383	-0.646656
6	-0.697496	3.518592	0.307080
1	-1.429854	2.287962	-1.337431
1	0.318739	2.415698	-1.272098
6	-0.786215	4.850488	-0.444267
1	-1.584235	3.381452	0.932957
1	0.167133	3.526508	0.979445

## S12

6	-0.906903	6.055456	0.493139
1	0.099287	4.970191	-1.080656
1	-1.648815	4.826418	-1.120955
1	-0.970834	6.992265	-0.068041
1	-1.801743	5.979798	1.118663
1	-0.041818	6.125084	1.160272

33

Bu-Br RCS=3.0

6	-0.340783	1.093486	-0.075895
6	-0.214721	-0.023210	0.428866
6	-0.915368	-1.188052	1.062605
6	-2.127326	-0.633677	1.895362
6	-1.313599	-2.184298	-0.034034
1	-0.433669	-2.465729	-0.619153
1	-1.722651	-3.083246	0.429144
1	-2.069630	-1.769027	-0.705078
6	-3.050215	-1.751836	2.391613
1	-3.738805	-1.351325	3.138199
1	-2.461689	-2.550013	2.852278
8	-0.091571	-1.821473	2.052250
1	0.712676	-2.134668	1.620003
53	2.293505	-0.351498	-0.099720
1	-1.663587	-0.142931	2.754069
1	-3.646963	-2.164367	1.576005
16	-3.080095	0.719509	1.088710
35	4.899628	-1.049820	-0.484406
1	-3.752228	-0.033283	0.108278
35	-4.819045	-1.174371	-1.477668
6	-0.334996	2.386935	-0.736855
6	-0.225637	3.587139	0.221753
1	-1.258133	2.451285	-1.324913
1	0.490622	2.398663	-1.459888
6	-0.249198	4.927678	-0.518698
1	-1.053662	3.538832	0.935392
1	0.699251	3.497555	0.801640
6	-0.145917	6.130088	0.424063
1	0.574776	4.958821	-1.242342
1	-1.173799	5.000685	-1.103746
1	-0.166797	7.073464	-0.129290
1	-0.975890	6.143572	1.137249
1	0.784639	6.101926	0.999855

33

Bu-Br RCS=3.2

6	-0.220397	1.132755	-0.132986
6	-0.294282	0.043685	0.418218
6	-1.028856	-1.087454	1.063173
6	-2.229650	-0.494389	1.892728
6	-1.455306	-2.087034	-0.017575
1	-0.585052	-2.400867	-0.601557
1	-1.887885	-2.966588	0.460373
1	-2.203179	-1.660666	-0.690957
6	-3.168422	-1.591670	2.403484
1	-3.843321	-1.168416	3.149895
1	-2.595260	-2.399528	2.868182
8	-0.217613	-1.728796	2.062787
1	0.567745	-2.084607	1.629532
53	2.299321	-0.417684	-0.111441
1	-1.750123	-0.004760	2.743330
1	-3.779195	-1.996954	1.594495
16	-3.168947	0.871559	1.082671
35	4.828470	-1.272710	-0.441790
1	-3.858939	0.119319	0.126767
35	-4.943577	-1.095867	-1.454516
6	-0.125475	2.424538	-0.790660
6	0.125377	3.603162	0.169404
1	-1.072967	2.567544	-1.325562
1	0.655588	2.384103	-1.558017
6	0.159337	4.949474	-0.560197
1	-0.661128	3.611007	0.930387

### S13

1	1.072980	3.440136	0.694297
6	0.403831	6.132073	0.382583
1	0.941290	4.927584	-1.329341
1	-0.788820	5.096172	-1.090973
1	0.422233	7.079628	-0.163852
1	-0.382511	6.199276	1.140810
1	1.360335	6.029660	0.905228

33

Bu-Br RCS=3.4

6	0.028976	1.233143	-0.146672
6	-0.490462	0.289412	0.421241
6	-1.343148	-0.724598	1.088345
6	-2.490634	0.043302	1.823965
6	-1.835296	-1.753116	0.063013
1	-0.984653	-2.187296	-0.470378
1	-2.366470	-2.551208	0.582652
1	-2.522284	-1.308686	-0.660997
6	-3.555219	-0.890258	2.402369
1	-4.208416	-0.320788	3.067040
1	-3.085322	-1.693531	2.977460
8	-0.610387	-1.369167	2.149606
1	0.105630	-1.880630	1.753900
53	2.187542	-0.627337	-0.104354
1	-1.989210	0.571014	2.638921
1	-4.177264	-1.319167	1.614208
16	-3.228822	1.399387	0.812031
35	4.512871	-1.912657	-0.365579
1	-4.031422	0.611952	-0.012887
35	-5.320059	-0.757564	-1.347363
6	0.439648	2.465510	-0.812382
6	1.296347	3.399662	0.062271
1	-0.487273	2.974278	-1.106389
1	0.972533	2.223484	-1.738393
6	1.674085	4.694187	-0.664292
1	0.741772	3.634087	0.976871
1	2.203360	2.869998	0.371712
6	2.522307	5.635211	0.196153
1	2.220547	4.447579	-1.582859
1	0.760747	5.212032	-0.981190
1	2.778210	6.549852	-0.346600
1	1.988270	5.926409	1.106119
1	3.457718	5.155651	0.501140

33

Bu-Br RCS=3.6

6	0.149509	1.281075	-0.203960
6	-0.515170	0.435601	0.369431
6	-1.394986	-0.543059	1.054935
6	-2.542011	0.245043	1.766922
6	-1.888954	-1.597449	0.056804
1	-1.038654	-2.056978	-0.455471
1	-2.435302	-2.373013	0.594112
1	-2.564411	-1.168350	-0.686162
6	-3.579174	-0.674399	2.414484
1	-4.230598	-0.079489	3.058384
1	-3.085806	-1.437253	3.023460
8	-0.668880	-1.163729	2.137236
1	0.032553	-1.706827	1.757835
53	2.190468	-0.666185	-0.103959
1	-2.038330	0.825983	2.543515
1	-4.208121	-1.154934	1.662342
16	-3.327471	1.528027	0.695830
35	4.430773	-2.086747	-0.296292
1	-4.135505	0.680453	-0.060420
35	-5.448464	-0.786536	-1.269051
6	0.665140	2.470329	-0.882941
6	1.543267	3.369424	0.006931
1	-0.211466	3.031624	-1.229771
1	1.221937	2.172285	-1.777711
6	2.036149	4.617881	-0.731279

S14

1	0.967005	3.662612	0.890750
1	2.399497	2.790570	0.368513
6	2.905323	5.524773	0.144804
1	2.605109	4.312932	-1.618125
1	1.173375	5.184984	-1.101297
1	3.243810	6.406776	-0.406693
1	2.352075	5.873050	1.022674
1	3.793245	4.994381	0.502922

33

Bu-Br RCS=3.8

6	0.273595	1.358222	-0.273919
6	-0.494532	0.600770	0.295438
6	-1.428596	-0.319182	0.993782
6	-2.575957	0.510446	1.660749
6	-1.927889	-1.400309	0.027616
1	-1.079252	-1.912213	-0.435420
1	-2.522644	-2.130157	0.576705
1	-2.561631	-0.981012	-0.755266
6	-3.577527	-0.373718	2.408834
1	-4.227628	0.261868	3.014023
1	-3.055502	-1.072564	3.067582
8	-0.733930	-0.914670	2.112443
1	-0.049320	-1.499334	1.765599
53	2.181578	-0.718717	-0.098602
1	-2.070185	1.165099	2.374962
1	-4.213426	-0.927299	1.714985
16	-3.430163	1.679544	0.512803
35	4.316717	-2.282574	-0.212283
1	-4.247341	0.752812	-0.130322
35	-5.583254	-0.844860	-1.149509
6	0.911280	2.485628	-0.958951
6	1.816552	3.337679	-0.049963
1	0.101645	3.105590	-1.363091
1	1.484518	2.120300	-1.817539
6	2.443072	4.521211	-0.793768
1	1.225423	3.700917	0.797329
1	2.605151	2.703142	0.367584
6	3.340061	5.381208	0.101385
1	3.027012	4.146499	-1.643347
1	1.647541	5.144289	-1.220336
1	3.774416	6.217258	-0.454469
1	2.775797	5.797428	0.941856
1	4.164268	4.792510	0.516161

33

Bu-Br RCS=4.0

6	0.416962	1.446890	-0.352527
6	-0.441940	0.771699	0.191678
6	-1.450584	-0.074830	0.883483
6	-2.595679	0.815607	1.482827
6	-1.957835	-1.173078	-0.058192
1	-1.118416	-1.770603	-0.425881
1	-2.652064	-1.823204	0.473101
1	-2.491520	-0.750738	-0.909464
6	-3.563036	0.005086	2.352909
1	-4.216077	0.697637	2.888368
1	-3.016049	-0.599973	3.079169
8	-0.813540	-0.651584	2.046343
1	-0.143315	-1.275691	1.742991
53	2.164871	-0.776617	-0.095300
1	-2.087411	1.554780	2.107191
1	-4.201001	-0.638520	1.743600
16	-3.519760	1.831305	0.242823
35	4.174574	-2.487966	-0.116362
1	-4.354903	0.825631	-0.234650
35	-5.726175	-0.912332	-0.965903
6	1.185464	2.501177	-1.021901
6	2.114889	3.289546	-0.080169
1	0.458487	3.182610	-1.480199
1	1.768500	2.069781	-1.842347

## S15

6	2.880644	4.398176	-0.808943
1	1.516087	3.720271	0.729323
1	2.821979	2.597246	0.388313
6	3.802574	5.195712	0.118132
1	3.472278	3.956222	-1.619991
1	2.166092	5.079039	-1.287528
1	4.336773	5.978806	-0.427742
1	3.234741	5.677166	0.920487
1	4.549417	4.546541	0.585749

33

Bu-Br RCS=4.2

6	0.578362	1.537763	-0.436856
6	-0.363180	0.938888	0.058861
6	-1.463316	0.183979	0.721412
6	-2.598507	1.161308	1.211997
6	-1.977724	-0.929269	-0.198247
1	-1.175043	-1.642551	-0.408414
1	-2.814167	-1.450733	0.266842
1	-2.335038	-0.517546	-1.141464
6	-3.531288	0.494907	2.231557
1	-4.206453	1.255136	2.630089
1	-2.962397	0.055517	3.052285
8	-0.917616	-0.368757	1.940452
1	-0.277621	-1.048924	1.698957
53	2.127706	-0.836758	-0.099407
1	-2.085629	1.997000	1.694640
1	-4.149918	-0.273212	1.762608
16	-3.590097	1.955881	-0.138317
35	3.993475	-2.691518	-0.018994
1	-4.437857	0.883248	-0.388483
35	-5.828482	-0.989807	-0.707023
6	1.479760	2.512914	-1.059687
6	2.418021	3.219242	-0.063016
1	0.850835	3.256078	-1.564681
1	2.070696	2.024101	-1.841339
6	3.327837	4.246307	-0.744224
1	1.812875	3.709752	0.706811
1	3.026698	2.467806	0.450261
6	4.260564	4.961641	0.237463
1	3.925056	3.745017	-1.515692
1	2.711336	4.987178	-1.268087
1	4.898417	5.687509	-0.275180
1	3.691363	5.499777	1.001931
1	4.912979	4.249316	0.751954

33

Bu-Br RCS=4.4

6	0.713396	1.601515	-0.505797
6	-0.295545	1.069514	-0.067427
6	-1.469557	0.395532	0.559499
6	-2.597919	1.443706	0.932790
6	-1.980337	-0.745324	-0.327797
1	-1.214887	-1.522387	-0.416019
1	-2.892718	-1.176148	0.088614
1	-2.218722	-0.377835	-1.325375
6	-3.484185	0.944844	2.082778
1	-4.187135	1.739021	2.342468
1	-2.886839	0.691594	2.959175
8	-1.007576	-0.116356	1.829700
1	-0.413814	-0.855227	1.651406
53	2.083908	-0.874368	-0.112879
1	-2.083788	2.353195	1.252944
1	-4.072634	0.075442	1.781797
16	-3.667855	2.006428	-0.479476
35	3.820508	-2.838879	0.048036
1	-4.500126	0.895671	-0.516883
35	-5.846893	-1.054812	-0.459785
6	1.717745	2.511772	-1.067491
6	2.646957	3.139785	-0.011474
1	1.176999	3.303593	-1.599979

## S16

1	2.315295	1.985580	-1.819265
6	3.668876	4.099656	-0.628586
1	2.036804	3.669350	0.727948
1	3.166983	2.341493	0.527707
6	4.594911	4.735629	0.412330
1	4.270020	3.559830	-1.370417
1	3.140984	4.888684	-1.178381
1	5.313728	5.414799	-0.055165
1	4.024913	5.309791	1.149506
1	5.161518	3.972463	0.954770

33

Bu-Br RCS=4.6

6	0.814127	1.643687	-0.565688
6	-0.243527	1.154727	-0.195125
6	-1.480516	0.538756	0.372246
6	-2.599201	1.646077	0.636975
6	-1.974699	-0.616509	-0.504747
1	-1.225333	-1.414131	-0.528449
1	-2.917686	-1.010975	-0.116906
1	-2.151599	-0.276449	-1.524534
6	-3.412876	1.344569	1.904038
1	-4.123204	2.159883	2.054865
1	-2.768054	1.260338	2.779371
8	-1.107415	0.047093	1.678131
1	-0.609327	-0.768672	1.551826
53	2.052153	-0.895116	-0.132300
1	-2.079774	2.597682	0.771339
1	-3.986976	0.422417	1.792458
16	-3.768497	1.984228	-0.774464
35	3.697893	-2.927001	0.088927
1	-4.566898	0.861374	-0.605109
35	-5.813916	-1.113631	-0.199034
6	1.893125	2.512148	-1.050701
6	2.782897	3.080993	0.070976
1	1.426329	3.336671	-1.603235
1	2.511588	1.967513	-1.771776
6	3.884559	4.000043	-0.466047
1	2.153128	3.628220	0.780468
1	3.230846	2.251546	0.627394
6	4.772894	4.576530	0.640278
1	4.504750	3.442787	-1.178741
1	3.429082	4.821015	-1.033677
1	5.550185	5.227274	0.229337
1	4.185710	5.166599	1.350917
1	5.268527	3.779638	1.203241

33

Bu-Br RCS=4.8

6	0.585092	1.658758	-0.654043
6	-0.344063	0.899352	-0.463102
6	-1.699909	0.316923	-0.431559
6	-2.600579	1.635995	-0.480151
6	-1.876716	-0.614814	-1.643490
1	-1.119578	-1.399840	-1.592858
1	-2.864652	-1.073344	-1.601055
1	-1.779911	-0.072453	-2.586258
6	-2.831554	2.207197	0.920907
1	-3.301584	3.190210	0.841278
1	-1.885437	2.305475	1.462205
8	-1.849950	-0.395690	0.774876
1	-2.762328	-0.775365	0.815292
53	1.974371	-0.857461	-0.172721
1	-2.050539	2.367406	-1.075687
1	-3.484711	1.553798	1.500076
16	-4.147343	1.483555	-1.437223
35	3.842703	-2.697685	0.085477
1	-4.725031	0.508637	-0.658423
35	-5.002851	-1.388969	0.862790
6	1.619298	2.673208	-0.849674
6	2.246290	3.183968	0.462074



## S17

1	1.162371	3.513874	-1.388738
1	2.402720	2.277013	-1.505347
6	3.313700	4.256088	0.222839
1	1.453114	3.582676	1.103282
1	2.684043	2.336217	0.998077
6	3.941152	4.772742	1.520919
1	4.099114	3.846333	-0.423981
1	2.870604	5.095504	-0.327805
1	4.699936	5.535112	1.321582
1	3.184951	5.217896	2.175104
1	4.421241	3.961334	2.076353

33

Bu-Br RCS=5.0

6	0.638003	1.706108	-0.691906
6	-0.353167	1.014504	-0.566694
6	-1.706658	0.417838	-0.540126
6	-2.652450	1.687253	-0.695690
6	-1.842878	-0.590116	-1.695121
1	-1.065240	-1.349676	-1.597639
1	-2.818160	-1.072466	-1.636350
1	-1.753193	-0.098425	-2.666903
6	-2.784714	2.451209	0.624474
1	-3.315134	3.390689	0.454345
1	-1.800633	2.670196	1.051324
8	-1.855384	-0.215757	0.711240
1	-2.750012	-0.633645	0.778460
53	1.948870	-0.853179	-0.206838
1	-2.184973	2.333750	-1.443276
1	-3.343296	1.862589	1.352591
16	-4.290477	1.349371	-1.455334
35	3.758814	-2.736876	0.075379
1	-4.722124	0.419550	-0.534629
35	-4.917206	-1.398104	1.029185
6	1.724975	2.677091	-0.822975
6	2.308153	3.141346	0.525713
1	1.333568	3.544563	-1.370299
1	2.522383	2.254549	-1.444173
6	3.431058	4.169100	0.355600
1	1.502511	3.565335	1.134332
1	2.682402	2.268162	1.068873
6	4.016915	4.638695	1.690489
1	4.228428	3.734860	-0.259904
1	3.051595	5.035099	-0.201442
1	4.816055	5.370545	1.540378
1	3.249743	5.106025	2.315793
1	4.434954	3.799041	2.254040

33

Bu-Br RCS=5.2

6	0.711138	1.778826	-0.732349
6	-0.354876	1.195707	-0.665032
6	-1.716461	0.596547	-0.626554
6	-2.722140	1.816855	-0.769008
6	-1.854899	-0.416769	-1.777803
1	-1.059905	-1.160321	-1.703397
1	-2.817882	-0.920202	-1.698189
1	-1.798304	0.079604	-2.750273
6	-2.751764	2.668167	0.502835
1	-3.359012	3.560621	0.338345
1	-1.741206	2.975764	0.792407
8	-1.820124	-0.033604	0.633097
1	-2.679694	-0.517878	0.717153
53	1.882366	-0.858188	-0.245907
1	-2.362741	2.422793	-1.606233
1	-3.180678	2.102060	1.329989
16	-4.439945	1.369920	-1.314705
35	3.598178	-2.814389	0.045719
1	-4.698323	0.412212	-0.356491
35	-4.739184	-1.479442	1.103952
6	1.871178	2.670129	-0.808377

## S18

6	2.413952	3.095097	0.569771
1	1.573011	3.561459	-1.375115
1	2.668367	2.188933	-1.385296
6	3.617866	4.035817	0.461056
1	1.610494	3.579979	1.134274
1	2.692372	2.198840	1.132568
6	4.163697	4.466287	1.825804
1	4.412931	3.540782	-0.109924
1	3.334973	4.925316	-0.116103
1	5.022413	5.135722	1.719469
1	3.400709	4.992299	2.408177
1	4.486285	3.600197	2.411628

33

Bu-Br RCS=5.4

6	0.826950	1.925526	-0.797099
6	-0.320145	1.518168	-0.720923
6	-1.713750	0.956265	-0.650273
6	-2.750361	2.145421	-0.458375
6	-1.983277	0.169763	-1.947435
1	-1.195592	-0.570526	-2.097391
1	-2.939835	-0.345910	-1.864224
1	-2.017944	0.839961	-2.810863
6	-2.574362	2.817253	0.904636
1	-3.226746	3.689266	0.981613
1	-1.536575	3.138712	1.048445
8	-1.689104	0.103471	0.479149
1	-2.509826	-0.449175	0.530415
53	1.677596	-0.919945	-0.234026
1	-2.550208	2.869965	-1.253709
1	-2.825533	2.121561	1.705795
16	-4.569259	1.727951	-0.753668
35	3.261504	-2.965056	0.024115
1	-4.623974	0.559268	-0.023844
35	-4.440827	-1.650894	0.873641
6	2.118663	2.609138	-0.886245
6	2.694684	3.019693	0.482780
1	1.990153	3.501104	-1.512495
1	2.836873	1.966470	-1.407310
6	4.044618	3.733337	0.361825
1	1.973708	3.668030	0.992303
1	2.801589	2.125013	1.103967
6	4.624243	4.149401	1.717086
1	4.755920	3.075440	-0.152284
1	3.932668	4.620048	-0.275155
1	5.587775	4.654641	1.601739
1	3.949722	4.833262	2.242012
1	4.778954	3.279423	2.362520

31

Ph-Br 1ec

6	-0.749555	5.037158	0.602361
6	-1.677676	4.252342	-0.081886
6	-1.546405	2.867709	-0.116835
6	-0.467959	2.259593	0.554447
6	0.461509	3.051059	1.250043
6	0.319746	4.433544	1.266865
1	-0.857717	6.116515	0.619975
1	-2.514671	4.714169	-0.593440
1	-2.277999	2.246680	-0.631022
1	1.291366	2.577440	1.760398
1	1.043584	5.040873	1.799206
6	-0.385114	0.835776	0.528458
6	-0.474410	-0.381547	0.470807
6	-1.007704	-1.769728	0.362353
6	-2.392574	-1.731775	1.091629
6	-1.119186	-2.118147	-1.128566
1	-0.142960	-2.013697	-1.610917
1	-1.462863	-3.148227	-1.221870
1	-1.835164	-1.451855	-1.617569
6	-2.249815	-1.611608	2.609516

## S19

1	-3.230579	-1.435945	3.054518
1	-1.595985	-0.774217	2.869640
8	-0.180618	-2.708718	1.056585
1	0.672455	-2.745063	0.608072
53	2.297336	-0.230034	-0.073592
1	-2.931905	-0.873832	0.682575
1	-1.822797	-2.517686	3.043710
16	-3.487660	-3.168042	0.678189
35	4.870756	-0.620407	-0.585363
1	-4.183688	-2.489764	-0.267010
35	-4.211542	0.350651	-1.367630
31			
Ph-Br 1ts			
6	-0.652373	4.897159	1.120492
6	-1.457452	4.238487	0.191732
6	-1.402042	2.854099	0.060429
6	-0.527466	2.118562	0.880774
6	0.278055	2.783624	1.822422
6	0.215515	4.166783	1.935597
1	-0.700258	5.977163	1.212988
1	-2.138817	4.800060	-0.437592
1	-2.042032	2.326701	-0.645192
1	0.951304	2.210177	2.448461
1	0.842566	4.676344	2.659045
6	-0.499905	0.697878	0.759957
6	-0.581043	-0.514780	0.644217
6	-1.003412	-1.937219	0.591674
6	-2.371199	-2.035216	1.418431
6	-1.098717	-2.394003	-0.868975
1	-0.102813	-2.360080	-1.320529
1	-1.477326	-3.415961	-0.904087
1	-1.762173	-1.745259	-1.443455
6	-2.314896	-3.081474	2.538727
1	-3.252119	-3.047030	3.098821
1	-1.485674	-2.883217	3.218117
8	-0.040014	-2.748103	1.292800
1	0.809627	-2.638939	0.847675
53	2.179813	-0.233125	-0.102391
1	-2.536440	-1.060175	1.874366
1	-2.187188	-4.089724	2.139229
16	-3.888817	-2.388838	0.426380
35	4.729063	-0.513325	-0.765375
1	-3.890479	-1.248553	-0.351630
35	-3.744134	0.636095	-1.826249
31			
Ph-Br 1r			
6	-0.398706	4.759820	0.286415
6	0.125609	3.891012	-0.669222
6	-0.032188	2.514846	-0.532883
6	-0.713534	1.977997	0.569521
6	-1.248241	2.864016	1.518625
6	-1.087749	4.239638	1.381141
1	-0.271963	5.831686	0.178929
1	0.662174	4.282949	-1.526167
1	0.376832	1.849265	-1.281113
1	-1.782149	2.466221	2.373742
1	-1.499117	4.905433	2.132441
6	-0.880117	0.519108	0.725225
6	-0.022590	-0.493759	0.537092
6	-0.614153	-1.898203	0.690723
6	-1.839508	-1.735616	1.628887
6	-0.959269	-2.465372	-0.695414
1	-0.059254	-2.479651	-1.313213
1	-1.326557	-3.489762	-0.600404
1	-1.713724	-1.858647	-1.202322
6	-2.899508	-2.828341	1.583413
1	-3.670666	-2.652370	2.338449
1	-2.430234	-3.791728	1.800860
8	0.251433	-2.808135	1.375325

S20

1	1.159327	-2.628696	1.085026
53	2.091487	-0.367685	0.016449
1	-1.426432	-1.666678	2.637380
1	-3.387542	-2.890807	0.609153
16	-2.522507	-0.055862	1.268703
35	5.112261	-0.326732	-0.721151
1	-3.823260	-0.233090	-0.494440
35	-4.823343	-0.326662	-1.594653

31

Ph-Br RCS=1.8

6	-0.385937	4.750289	0.289928
6	0.121706	3.880111	-0.673424
6	-0.042138	2.504608	-0.537089
6	-0.712886	1.969992	0.572589
6	-1.231023	2.857308	1.529480
6	-1.064356	4.232308	1.392265
1	-0.254300	5.821582	0.182615
1	0.650105	4.270430	-1.536157
1	0.354011	1.837752	-1.291140
1	-1.756421	2.461319	2.390733
1	-1.462354	4.899212	2.149762
6	-0.886969	0.510361	0.727916
6	-0.024102	-0.499292	0.535937
6	-0.614878	-1.904208	0.688253
6	-1.841284	-1.739206	1.624205
6	-0.958716	-2.471673	-0.698047
1	-0.057854	-2.486952	-1.314566
1	-1.327317	-3.495660	-0.603344
1	-1.711897	-1.864358	-1.206308
6	-2.908731	-2.824075	1.573520
1	-3.681697	-2.643325	2.325607
1	-2.447246	-3.790967	1.792125
8	0.249596	-2.814221	1.374119
1	1.158112	-2.632866	1.086951
53	2.087704	-0.369304	0.015975
1	-1.430396	-1.674593	2.633927
1	-3.393208	-2.882503	0.597252
16	-2.510035	-0.052659	1.265190
35	5.112086	-0.322734	-0.722613
1	-3.822248	-0.223180	-0.494373
35	-4.826540	-0.313426	-1.590215

31

Ph-Br RCS=2.0

6	-0.463548	4.832155	0.244038
6	0.162880	3.974051	-0.658325
6	0.042918	2.594507	-0.519728
6	-0.702738	2.043608	0.535072
6	-1.338753	2.918928	1.430805
6	-1.216581	4.297371	1.288851
1	-0.367678	5.906864	0.133158
1	0.748935	4.377033	-1.476905
1	0.531903	1.937499	-1.226188
1	-1.924880	2.507715	2.243959
1	-1.709861	4.954851	1.996843
6	-0.819258	0.591519	0.694807
6	-0.009213	-0.449381	0.538207
6	-0.614262	-1.847324	0.697355
6	-1.833818	-1.697601	1.648685
6	-0.968199	-2.407160	-0.689780
1	-0.072726	-2.418461	-1.314364
1	-1.332943	-3.432327	-0.596094
1	-1.726717	-1.798896	-1.187572
6	-2.839848	-2.843663	1.638353
1	-3.598538	-2.698920	2.412128
1	-2.317863	-3.781083	1.848749
8	0.252970	-2.762500	1.372962
1	1.157500	-2.601124	1.062817
53	2.126327	-0.357975	0.018387
1	-1.407460	-1.598470	2.648843

S21

1	-3.350241	-2.935838	0.677890
16	-2.613666	-0.067215	1.283167
35	5.116827	-0.374423	-0.701376
1	-3.847983	-0.301017	-0.473699
35	-4.833380	-0.425913	-1.593724

31

Ph-Br RCS=2.2

6	-0.476110	4.907659	0.179920
6	0.191681	4.056632	-0.699161
6	0.095617	2.676112	-0.553922
6	-0.667108	2.119862	0.487591
6	-1.343835	2.987280	1.360970
6	-1.245831	4.365862	1.209583
1	-0.400477	5.983228	0.062160
1	0.790703	4.465939	-1.505120
1	0.618231	2.021810	-1.238755
1	-1.946625	2.565584	2.155960
1	-1.772786	5.019121	1.896771
6	-0.742414	0.677265	0.653707
6	-0.002161	-0.400163	0.533769
6	-0.633181	-1.786010	0.689839
6	-1.850055	-1.640469	1.650589
6	-0.995389	-2.328341	-0.702122
1	-0.101884	-2.344113	-1.329709
1	-1.370183	-3.350258	-0.615818
1	-1.749117	-1.707925	-1.190887
6	-2.803796	-2.833484	1.671129
1	-3.548387	-2.715633	2.462498
1	-2.235703	-3.745810	1.872024
8	0.225974	-2.715385	1.356275
1	1.126819	-2.584658	1.023102
53	2.166247	-0.353503	0.020650
1	-1.413356	-1.514646	2.643171
1	-3.334739	-2.951519	0.724703
16	-2.716420	-0.058419	1.287795
35	5.113241	-0.454267	-0.669322
1	-3.879892	-0.353992	-0.415137
35	-4.859049	-0.523074	-1.558840

31

Ph-Br RCS=2.4

6	-0.448190	4.973436	0.096871
6	0.124838	4.119581	-0.844173
6	0.041252	2.740102	-0.684451
6	-0.610695	2.193024	0.434938
6	-1.191801	3.062289	1.373290
6	-1.108395	4.438850	1.204560
1	-0.384917	6.048369	-0.033061
1	0.638378	4.526287	-1.708250
1	0.490764	2.077291	-1.412382
1	-1.715469	2.640247	2.222085
1	-1.561414	5.097607	1.937442
6	-0.657708	0.761906	0.609080
6	-0.011956	-0.356973	0.522909
6	-0.677315	-1.725870	0.660250
6	-1.897140	-1.577933	1.623881
6	-1.043185	-2.237575	-0.741777
1	-0.147910	-2.261814	-1.367053
1	-1.438092	-3.252817	-0.671517
1	-1.784518	-1.596578	-1.221707
6	-2.814653	-2.802126	1.655957
1	-3.547532	-2.705550	2.460490
1	-2.217499	-3.698874	1.842014
8	0.163847	-2.678266	1.316973
1	1.060267	-2.586080	0.961502
53	2.202082	-0.354482	0.025628
1	-1.455051	-1.441578	2.612756
1	-3.360857	-2.928894	0.719566
16	-2.821877	-0.026595	1.283350
35	5.093612	-0.552536	-0.621615

S22

1	-3.874601	-0.371290	-0.293918
35	-4.859411	-0.602875	-1.491060

31  
Ph-Br RCS=2.6

6	-1.439925	4.750422	0.391261
6	-2.004849	3.861778	-0.525412
6	-1.766324	2.497298	-0.419805
6	-0.956245	2.011909	0.624714
6	-0.404266	2.909265	1.556750
6	-0.638825	4.272789	1.429814
1	-1.626102	5.815066	0.298583
1	-2.635964	4.230921	-1.325658
1	-2.221819	1.795976	-1.112120
1	0.215486	2.526193	2.358184
1	-0.199344	4.963356	2.140880
6	-0.695262	0.614932	0.726899
6	-0.057549	-0.472865	0.614380
6	-0.525901	-1.912285	0.719146
6	-1.764919	-1.979624	1.677297
6	-0.809260	-2.429217	-0.699007
1	0.082666	-2.308823	-1.318220
1	-1.052772	-3.492116	-0.654842
1	-1.634587	-1.889290	-1.170102
6	-2.525585	-3.306484	1.591206
1	-3.246589	-3.378323	2.407953
1	-1.822464	-4.139359	1.676098
8	0.439768	-2.741789	1.372068
1	1.289822	-2.620802	0.926081
53	2.193362	-0.160661	-0.032374
1	-1.345485	-1.874091	2.680068
1	-3.072184	-3.395644	0.650994
16	-2.883354	-0.531995	1.537339
35	4.949871	-0.108750	-0.740730
1	-3.385888	-0.675279	0.202353
35	-4.133984	-0.505650	-1.766180

31  
Ph-Br RCS=2.8

6	-1.731683	4.671068	0.503335
6	-2.198244	3.766760	-0.452011
6	-1.844919	2.425007	-0.382250
6	-1.019630	1.980158	0.670276
6	-0.567587	2.892535	1.643032
6	-0.915486	4.233093	1.549043
1	-2.007543	5.718199	0.437364
1	-2.844840	4.103587	-1.254050
1	-2.231605	1.706874	-1.100207
1	0.061540	2.538149	2.450427
1	-0.555701	4.937189	2.290929
6	-0.655828	0.612728	0.739784
6	-0.085046	-0.496374	0.641266
6	-0.491636	-1.950871	0.710175
6	-1.715415	-2.101758	1.679543
6	-0.768790	-2.435567	-0.720481
1	0.115219	-2.271781	-1.341470
1	-0.980734	-3.505866	-0.704616
1	-1.611207	-1.905053	-1.172864
6	-2.368055	-3.485995	1.591273
1	-3.068774	-3.617376	2.418024
1	-1.603375	-4.264870	1.655204
8	0.518065	-2.755729	1.329437
1	1.350141	-2.607603	0.859749
53	2.223661	-0.088328	-0.029166
1	-1.292236	-1.974723	2.678551
1	-2.923829	-3.607151	0.659907
16	-2.952803	-0.748227	1.583413
35	4.922750	-0.005569	-0.735265
1	-3.364870	-0.843534	0.245389
35	-3.997664	-0.462199	-1.881437

S23

31  
Ph-Br RCS=3.0

6	-1.766008	4.663122	0.600725
6	-2.238947	3.761591	-0.353466
6	-1.853255	2.427006	-0.313953
6	-0.989453	1.988219	0.709896
6	-0.529336	2.897287	1.682150
6	-0.910239	4.230225	1.617096
1	-2.067514	5.704436	0.557768
1	-2.916616	4.093059	-1.131758
1	-2.245033	1.710007	-1.031791
1	0.129417	2.546597	2.467314
1	-0.546577	4.932335	2.359013
6	-0.610434	0.625952	0.753234
6	-0.154589	-0.523372	0.673940
6	-0.526759	-1.980336	0.705533
6	-1.743927	-2.187028	1.674126
6	-0.796831	-2.434308	-0.736576
1	0.086255	-2.246741	-1.352435
1	-0.998218	-3.506574	-0.746066
1	-1.642286	-1.899540	-1.179066
6	-2.328151	-3.601130	1.573369
1	-3.019305	-3.770182	2.401319
1	-1.529817	-4.346557	1.625740
8	0.506256	-2.776245	1.302878
1	1.326494	-2.615529	0.817971
53	2.236181	-0.064774	-0.028164
1	-1.324226	-2.051714	2.673662
1	-2.884077	-3.737425	0.644085
16	-3.052136	-0.895157	1.604304
35	4.885296	-0.006793	-0.735312
1	-3.389044	-0.931143	0.257529
35	-3.914591	-0.368033	-1.964086

31  
Ph-Br RCS=3.2

6	-1.538991	4.724739	0.684784
6	-2.108176	3.841845	-0.233016
6	-1.775333	2.491848	-0.213976
6	-0.865297	2.020412	0.752448
6	-0.304106	2.910499	1.686610
6	-0.635890	4.257887	1.643275
1	-1.800390	5.777408	0.658065
1	-2.819826	4.198996	-0.968580
1	-2.236189	1.792080	-0.908513
1	0.392055	2.535700	2.427240
1	-0.195986	4.944794	2.357755
6	-0.555745	0.637100	0.777050
6	-0.280684	-0.558404	0.714117
6	-0.641576	-2.007975	0.694654
6	-1.862253	-2.252903	1.649248
6	-0.900655	-2.420021	-0.762251
1	-0.010551	-2.220384	-1.364317
1	-1.109618	-3.489914	-0.804040
1	-1.736378	-1.864287	-1.198065
6	-2.424762	-3.672293	1.510496
1	-3.119294	-3.867320	2.329983
1	-1.618842	-4.410614	1.550404
8	0.397589	-2.815043	1.274210
1	1.211745	-2.653364	0.780393
53	2.234708	-0.092833	-0.029017
1	-1.449615	-2.136787	2.654135
1	-2.975054	-3.792746	0.575652
16	-3.191734	-0.976672	1.606084
35	4.837580	-0.108559	-0.739972
1	-3.457414	-0.925755	0.250444
35	-3.873761	-0.195926	-2.006152

31  
Ph-Br RCS=3.4

6	-1.202885	4.791951	0.754384
---	-----------	----------	----------

S24

6	-1.889990	3.946869	-0.116783
6	-1.647561	2.576971	-0.111725
6	-0.705659	2.047768	0.790790
6	-0.021254	2.899668	1.674821
6	-0.267676	4.266444	1.649019
1	-1.395285	5.859628	0.739717
1	-2.623544	4.348984	-0.806342
1	-2.193909	1.909670	-0.775892
1	0.701689	2.482282	2.365471
1	0.266152	4.922785	2.327491
6	-0.498007	0.640343	0.799635
6	-0.426044	-0.578482	0.749391
6	-0.788233	-2.018173	0.670893
6	-2.015092	-2.302786	1.603858
6	-1.032840	-2.377929	-0.802708
1	-0.133324	-2.166072	-1.386510
1	-1.252546	-3.443246	-0.884500
1	-1.855423	-1.795808	-1.229363
6	-2.568617	-3.719094	1.413607
1	-3.271464	-3.941069	2.219218
1	-1.761213	-4.456701	1.439374
8	0.251462	-2.844136	1.230277
1	1.062711	-2.681052	0.732556
53	2.228831	-0.142811	-0.030195
1	-1.612027	-2.217695	2.615654
1	-3.109540	-3.811744	0.470164
16	-3.352153	-1.029917	1.589622
35	4.796550	-0.253837	-0.744244
1	-3.548967	-0.877233	0.231905
35	-3.864992	0.014601	-2.003924

31

Ph-Br RCS=3.6

6	-0.940094	4.831528	0.812496
6	-1.712443	4.025365	-0.023388
6	-1.540921	2.644507	-0.031698
6	-0.581886	2.064361	0.819188
6	0.191079	2.876859	1.664839
6	0.012049	4.254892	1.655734
1	-1.078384	5.907652	0.809344
1	-2.457453	4.466741	-0.675761
1	-2.149555	2.009050	-0.672509
1	0.928880	2.421857	2.314876
1	0.613555	4.879901	2.306728
6	-0.451408	0.643369	0.812071
6	-0.539979	-0.572871	0.767646
6	-0.905389	-2.006139	0.644866
6	-2.132526	-2.335861	1.560539
6	-1.137107	-2.324351	-0.840692
1	-0.230917	-2.100146	-1.409474
1	-1.361294	-3.385669	-0.954944
1	-1.950916	-1.724100	-1.258970
6	-2.645543	-3.763739	1.344285
1	-3.351535	-4.014137	2.138909
1	-1.820166	-4.481076	1.369391
8	0.140065	-2.841016	1.186267
1	0.948838	-2.669129	0.687514
53	2.226419	-0.179961	-0.031539
1	-1.741526	-2.255771	2.577358
1	-3.174708	-3.856977	0.394258
16	-3.510877	-1.103611	1.552147
35	4.771804	-0.372941	-0.745985
1	-3.632296	-0.854303	0.200351
35	-3.862781	0.188725	-1.985311

31

Ph-Br RCS=3.8

6	-0.745812	4.853848	0.886565
6	-1.560296	4.090368	0.050576
6	-1.446222	2.703671	0.023674
6	-0.501687	2.073704	0.854485



S25

6	0.315068	2.843058	1.698478
6	0.191765	4.227517	1.710106
1	-0.839963	5.934674	0.898658
1	-2.293721	4.570117	-0.587764
1	-2.086415	2.101415	-0.618518
1	1.042556	2.350625	2.332712
1	0.826513	4.818549	2.361336
6	-0.430887	0.645786	0.826667
6	-0.629607	-0.557462	0.776968
6	-0.997270	-1.987335	0.625935
6	-2.224586	-2.358789	1.525924
6	-1.211900	-2.283352	-0.866769
1	-0.296932	-2.056825	-1.420374
1	-1.441761	-3.341235	-0.999751
1	-2.014212	-1.669507	-1.287035
6	-2.658786	-3.815792	1.325778
1	-3.370872	-4.085878	2.108651
1	-1.800190	-4.490301	1.384073
8	0.055604	-2.819666	1.162141
1	0.865211	-2.632421	0.670181
53	2.215280	-0.206969	-0.032180
1	-1.857469	-2.243166	2.548010
1	-3.161504	-3.952535	0.366723
16	-3.681401	-1.214597	1.469424
35	4.744807	-0.461344	-0.748297
1	-3.690809	-0.854102	0.137986
35	-3.814275	0.344188	-1.983919

31

Ph-Br RCS=4.0

6	-0.757608	4.814390	1.298895
6	-1.415742	4.200666	0.233569
6	-1.370845	2.818957	0.073078
6	-0.657275	2.040996	1.001999
6	0.001067	2.660899	2.079446
6	-0.048796	4.041777	2.221891
1	-0.796502	5.892667	1.413757
1	-1.972382	4.796526	-0.481193
1	-1.893772	2.323484	-0.743857
1	0.550232	2.053297	2.789058
1	0.463284	4.516670	3.051654
6	-0.630880	0.623145	0.853214
6	-0.692627	-0.587802	0.720292
6	-1.034920	-2.031979	0.682569
6	-2.333180	-2.249944	1.533404
6	-1.137719	-2.528841	-0.764812
1	-0.150059	-2.492398	-1.231335
1	-1.489163	-3.561993	-0.772788
1	-1.813283	-1.905761	-1.354219
6	-2.541168	-3.719537	1.917908
1	-3.447850	-3.807283	2.522964
1	-1.694967	-4.090525	2.497374
8	-0.021591	-2.768703	1.401715
1	0.833056	-2.557659	1.004180
53	2.071516	-0.223642	-0.062125
1	-2.188626	-1.674361	2.449494
1	-2.671999	-4.348455	1.034956
16	-3.910416	-1.664658	0.750275
35	4.621446	-0.433581	-0.723465
1	-3.459484	-0.745788	-0.169616
35	-3.238626	0.597650	-2.220668

31

Ph-Br RCS=4.2

6	-0.601370	4.831813	1.321814
6	-1.322091	4.238613	0.285800
6	-1.315802	2.857053	0.117090
6	-0.576927	2.058182	1.007319
6	0.144873	2.657197	2.055126
6	0.132245	4.038163	2.206619
1	-0.610631	5.910019	1.443356

S26

1	-1.898221	4.850376	-0.399512
1	-1.887839	2.378565	-0.676737
1	0.713883	2.034019	2.734985
1	0.693319	4.496546	3.013705
6	-0.591136	0.639664	0.849586
6	-0.716171	-0.566002	0.713075
6	-1.065990	-2.008042	0.676163
6	-2.389736	-2.225514	1.498897
6	-1.139167	-2.515769	-0.769214
1	-0.139908	-2.497451	-1.211529
1	-1.508973	-3.542567	-0.777748
1	-1.794501	-1.888611	-1.375963
6	-2.525433	-3.666384	2.008067
1	-3.463057	-3.762990	2.562305
1	-1.697290	-3.924126	2.668042
8	-0.062100	-2.736364	1.418466
1	0.797970	-2.526533	1.032108
53	2.084132	-0.243494	-0.087086
1	-2.328216	-1.561206	2.362522
1	-2.551830	-4.380181	1.181764
16	-3.967032	-1.846621	0.601168
35	4.623771	-0.503860	-0.759507
1	-3.590233	-0.790479	-0.198427
35	-3.350168	0.718511	-2.112830

31

Ph-Br RCS=4.4

6	-0.463938	4.860688	1.285714
6	-1.252152	4.271463	0.297689
6	-1.272825	2.889052	0.136675
6	-0.491784	2.085084	0.985224
6	0.298268	2.679856	1.984391
6	0.311097	4.061774	2.129267
1	-0.452706	5.939471	1.401750
1	-1.860766	4.886818	-0.355596
1	-1.897576	2.415118	-0.619018
1	0.899903	2.053372	2.632329
1	0.924957	4.516591	2.899113
6	-0.538123	0.665010	0.833755
6	-0.732940	-0.532235	0.700932
6	-1.096964	-1.971101	0.663744
6	-2.445046	-2.186471	1.463498
6	-1.145643	-2.485216	-0.780260
1	-0.139423	-2.467657	-1.206837
1	-1.517116	-3.511404	-0.789301
1	-1.794344	-1.861993	-1.397446
6	-2.514599	-3.577464	2.109134
1	-3.469335	-3.679390	2.631783
1	-1.703291	-3.717931	2.822462
8	-0.102143	-2.697494	1.421303
1	0.761174	-2.498642	1.036410
53	2.108340	-0.259421	-0.104297
1	-2.464568	-1.437843	2.256778
1	-2.456246	-4.368215	1.357617
16	-4.011544	-2.013451	0.485627
35	4.638594	-0.577323	-0.783120
1	-3.738969	-0.880559	-0.252458
35	-3.488994	0.794297	-1.985134

31

Ph-Br RCS=4.6

6	-0.457720	4.900394	1.176909
6	-1.297676	4.280575	0.252241
6	-1.301784	2.895605	0.114112
6	-0.450937	2.119961	0.921500
6	0.391051	2.745562	1.857125
6	0.386364	4.129763	1.979429
1	-0.459711	5.980949	1.275396
1	-1.959956	4.873484	-0.368755
1	-1.966623	2.399008	-0.590874
1	1.046564	2.141559	2.473225

S27

1	1.040844	4.608371	2.699785
6	-0.485981	0.697469	0.791590
6	-0.682727	-0.501058	0.668628
6	-1.083034	-1.930421	0.622001
6	-2.455576	-2.092125	1.421847
6	-1.138634	-2.421872	-0.829366
1	-0.133236	-2.395082	-1.258750
1	-1.511634	-3.446818	-0.850721
1	-1.791425	-1.790144	-1.433474
6	-2.446442	-3.307562	2.359442
1	-3.400269	-3.348801	2.890840
1	-1.636820	-3.237634	3.085136
8	-0.105427	-2.695223	1.361190
1	0.754201	-2.545031	0.947632
53	2.153763	-0.259648	-0.108412
1	-2.580703	-1.194521	2.027253
1	-2.323592	-4.239565	1.803123
16	-3.989265	-2.256916	0.393321
35	4.685949	-0.601991	-0.780563
1	-3.891735	-1.091477	-0.341105
35	-3.672380	0.762611	-1.842532

31

Ph-Br RCS=4.8

6	-1.163430	4.940610	0.624970
6	-1.931127	4.113866	-0.194883
6	-1.693425	2.744097	-0.240715
6	-0.675578	2.193489	0.562832
6	0.087379	3.027982	1.401228
6	-0.153361	4.395328	1.421372
1	-1.352158	6.008710	0.648494
1	-2.725552	4.530919	-0.803332
1	-2.309445	2.086302	-0.850910
1	0.868965	2.596178	2.014670
1	0.443476	5.037129	2.059969
6	-0.468001	0.789244	0.531453
6	-0.313146	-0.424550	0.472751
6	-0.844766	-1.819281	0.431973
6	-2.207995	-1.699077	1.199763
6	-0.987753	-2.228980	-1.038792
1	-0.016938	-2.157410	-1.538569
1	-1.346474	-3.257125	-1.082832
1	-1.703063	-1.578822	-1.549329
6	-2.016887	-1.662036	2.717158
1	-2.963811	-1.405793	3.195594
1	-1.269775	-0.913848	2.996632
8	-0.018203	-2.738703	1.145148
1	0.816764	-2.819616	0.669454
53	2.303854	-0.169518	-0.083336
1	-2.672885	-0.776734	0.850915
1	-1.680108	-2.627564	3.098645
16	-3.436278	-2.977160	0.740096
35	4.913652	-0.418455	-0.611605
1	-4.013079	-2.205762	-0.226909
35	-4.137810	0.126681	-1.485625

31

Ph-Br RCS=5.0

6	-0.835881	5.019375	0.596810
6	-1.734479	4.220181	-0.109746
6	-1.578859	2.838081	-0.143390
6	-0.506807	2.247282	0.553362
6	0.392199	3.053411	1.272654
6	0.227403	4.433126	1.286396
1	-0.962550	6.096732	0.612800
1	-2.567262	4.668622	-0.639687
1	-2.288984	2.205544	-0.673243
1	1.216935	2.592584	1.802710
1	0.927944	5.052069	1.836194
6	-0.396727	0.826684	0.530126
6	-0.432138	-0.393638	0.473444

S28

6	-0.971106	-1.780334	0.379951
6	-2.349881	-1.712650	1.120270
6	-1.093219	-2.141580	-1.106607
1	-0.118356	-2.048551	-1.594299
1	-1.445318	-3.169748	-1.188357
1	-1.807243	-1.476177	-1.599441
6	-2.191446	-1.622963	2.638861
1	-3.161904	-1.417901	3.093913
1	-1.503576	-0.816435	2.908574
8	-0.149290	-2.720428	1.077145
1	0.698297	-2.772861	0.620046
53	2.303709	-0.219764	-0.075281
1	-2.863121	-0.830512	0.731415
1	-1.796815	-2.552072	3.054378
16	-3.495571	-3.094169	0.685295
35	4.884181	-0.580249	-0.591653
1	-4.154720	-2.372180	-0.258016
35	-4.207632	0.289867	-1.386968

31

Ph-Br RCS=5.2

6	-0.583299	5.060847	0.650633
6	-1.551488	4.320184	-0.027325
6	-1.476871	2.931660	-0.076156
6	-0.413847	2.274167	0.571897
6	0.556571	3.020993	1.259853
6	0.470031	4.408051	1.293367
1	-0.647760	6.143482	0.679960
1	-2.375997	4.820145	-0.523227
1	-2.238330	2.344327	-0.586730
1	1.374810	2.510391	1.752902
1	1.225287	4.980195	1.821101
6	-0.389568	0.846072	0.528724
6	-0.576146	-0.360130	0.463450
6	-1.084330	-1.757557	0.332060
6	-2.485192	-1.795796	1.028959
6	-1.162124	-2.093981	-1.164517
1	-0.181060	-1.966199	-1.630314
1	-1.481689	-3.130376	-1.274145
1	-1.881072	-1.433240	-1.657055
6	-2.394728	-1.585711	2.540726
1	-3.398527	-1.490329	2.957569
1	-1.839361	-0.670982	2.766257
8	-0.239994	-2.677702	1.034305
1	0.627895	-2.671012	0.613207
53	2.267649	-0.246453	-0.074418
1	-3.085228	-1.009031	0.562564
1	-1.886253	-2.418504	3.030922
16	-3.431089	-3.368597	0.689097
35	4.831009	-0.684910	-0.578162
1	-4.199323	-2.833782	-0.284801
35	-4.169165	0.501862	-1.364526

31

Ph-Br RCS=5.4

6	-0.332082	5.095724	0.675705
6	-1.351239	4.411855	0.012808
6	-1.349957	3.021756	-0.047911
6	-0.308784	2.303349	0.569130
6	0.713470	2.992960	1.239775
6	0.698792	4.382677	1.289359
1	-0.339775	6.179948	0.715730
1	-2.158933	4.958323	-0.461432
1	-2.150408	2.478512	-0.546829
1	1.515347	2.437351	1.710222
1	1.493678	4.909250	1.806318
6	-0.363388	0.872058	0.509542
6	-0.727150	-0.298409	0.446207
6	-1.208408	-1.715173	0.282421
6	-2.626481	-1.878412	0.939536
6	-1.241694	-2.027122	-1.221504

S29

1	-0.253684	-1.872748	-1.663102
1	-1.536260	-3.068367	-1.356309
1	-1.960088	-1.368446	-1.717162
6	-2.605320	-1.606055	2.442444
1	-3.622689	-1.619735	2.836074
1	-2.174779	-0.619681	2.637991
8	-0.334958	-2.607076	0.988107
1	0.544781	-2.544219	0.596312
53	2.238185	-0.268255	-0.068935
1	-3.288075	-1.171886	0.430744
1	-2.008613	-2.348769	2.976306
16	-3.410556	-3.583727	0.653582
35	4.785066	-0.815391	-0.556257
1	-4.224783	-3.178988	-0.342563
35	-4.127852	0.698589	-1.305342

39

Bu-NO3 1ec

6	-0.493394	0.665713	0.867910
6	-0.607472	-0.549234	0.700659
6	-1.320175	-1.874942	0.668705
6	-1.420435	-2.359735	-0.821975
6	-0.572449	-2.880781	1.556119
1	-0.459008	-2.461401	2.557026
1	-1.162122	-3.794177	1.618483
1	0.413300	-3.119337	1.153077
6	-2.029851	-1.324318	-1.768291
1	-2.105394	-1.741112	-2.773906
1	-1.403984	-0.428872	-1.817423
8	-2.600294	-1.704396	1.237281
1	-2.985409	-0.806157	1.051963
53	1.852141	-0.381893	0.099501
1	-0.412866	-2.619801	-1.158034
1	-3.028663	-1.020015	-1.446803
16	-2.334403	-3.967706	-0.929748
1	-3.455742	-3.510733	-0.334813
8	-4.687355	0.720860	-0.690020
8	3.964862	-0.823963	-0.574036
7	-3.999962	1.405724	0.088295
7	4.956846	-0.003044	-0.205082
8	-3.387520	0.831960	1.060332
8	-3.875463	2.638506	-0.048799
8	6.072949	-0.332944	-0.576408
8	4.688781	0.993972	0.455688
6	-0.520125	2.103578	1.081196
1	-1.506548	2.278750	1.532508
1	0.246742	2.383185	1.812172
6	-0.395253	2.946612	-0.202155
1	-1.181197	2.638504	-0.896600
1	0.570235	2.748326	-0.679840
6	-0.541256	4.442580	0.090271
1	-1.514959	4.613457	0.561019
1	0.223353	4.750932	0.815058
6	-0.426418	5.302410	-1.171544
1	-1.204922	5.038913	-1.893484
1	-0.534878	6.365935	-0.938393
1	0.544154	5.165190	-1.659744

39

Bu-NO3 1r

6	0.780809	0.376775	-1.061482
6	-0.134745	-0.468749	-0.579793
6	0.350386	-1.887283	-0.273088
6	1.595332	-2.098788	-1.176571
6	0.636229	-2.031059	1.229591
1	-0.269901	-1.803256	1.794475
1	0.935066	-3.055833	1.460211
1	1.421479	-1.344148	1.556717
6	2.577470	-3.186888	-0.767192
1	3.373992	-3.289804	-1.508334
1	2.046664	-4.140864	-0.705983

S30

8	-0.571061	-2.900209	-0.684874
1	-1.461754	-2.625064	-0.420213
53	-2.162057	0.028021	-0.120124
1	1.198440	-2.319003	-2.169448
1	3.043529	-2.986152	0.198754
16	2.383423	-0.428475	-1.345311
1	3.584967	-0.081489	0.429011
8	4.049434	0.239019	1.262212
8	-4.659851	0.778918	0.422115
7	5.289473	-0.369402	1.291386
7	-5.535886	-0.079836	0.800821
8	5.550244	-1.145657	0.393382
8	5.979313	-0.051807	2.226714
8	-6.692169	0.308724	1.041558
8	-5.205193	-1.279031	0.917523
6	0.668870	1.837510	-1.380611
1	1.113059	2.027163	-2.365803
1	-0.393526	2.085326	-1.453827
6	1.332528	2.757158	-0.337824
1	2.397689	2.511700	-0.246887
1	0.884544	2.558858	0.642075
6	1.184000	4.243422	-0.680166
1	1.624143	4.433401	-1.667336
1	0.118624	4.486242	-0.768503
6	1.834063	5.166103	0.355152
1	2.906920	4.967128	0.445074
1	1.711437	6.219184	0.084700
1	1.388367	5.022906	1.344311
6	0.780809	0.376775	-1.061482
6	-0.134745	-0.468749	-0.579793
6	0.350386	-1.887283	-0.273088
6	1.595332	-2.098788	-1.176571
6	0.636229	-2.031059	1.229591
1	-0.269901	-1.803256	1.794475
1	0.935066	-3.055833	1.460211
1	1.421479	-1.344148	1.556717
6	2.577470	-3.186888	-0.767192
1	3.373992	-3.289804	-1.508334
1	2.046664	-4.140864	-0.705983
8	-0.571061	-2.900209	-0.684874
1	-1.461754	-2.625064	-0.420213
53	-2.162057	0.028021	-0.120124
1	1.198440	-2.319003	-2.169448
1	3.043529	-2.986152	0.198754
16	2.383423	-0.428475	-1.345311
1	3.584967	-0.081489	0.429011
8	4.049434	0.239019	1.262212
8	-4.659851	0.778918	0.422115
7	5.289473	-0.369402	1.291386
7	-5.535886	-0.079836	0.800821
8	5.550244	-1.145657	0.393382
8	5.979313	-0.051807	2.226714
8	-6.692169	0.308724	1.041558
8	-5.205193	-1.279031	0.917523
6	0.668870	1.837510	-1.380611
1	1.113059	2.027163	-2.365803
1	-0.393526	2.085326	-1.453827
6	1.332528	2.757158	-0.337824
1	2.397689	2.511700	-0.246887
1	0.884544	2.558858	0.642075
6	1.184000	4.243422	-0.680166
1	1.624143	4.433401	-1.667336
1	0.118624	4.486242	-0.768503
6	1.834063	5.166103	0.355152
1	2.906920	4.967128	0.445074
1	1.711437	6.219184	0.084700
1	1.388367	5.022906	1.344311

39

Bu-NO3 RC=1.8

6	0.786735	0.363793	-1.060394
---	----------	----------	-----------

S31

6	-0.132924	-0.477077	-0.575607
6	0.351573	-1.893801	-0.260220
6	1.600028	-2.106987	-1.158298
6	0.632585	-2.030450	1.244028
1	-0.275658	-1.800989	1.804811
1	0.931837	-3.053802	1.480468
1	1.416066	-1.341164	1.570591
6	2.587756	-3.185629	-0.738036
1	3.388697	-3.287202	-1.474577
1	2.063474	-4.143024	-0.673850
8	-0.567399	-2.909657	-0.670485
1	-1.459362	-2.633247	-0.411478
53	-2.159946	0.023042	-0.122699
1	1.207401	-2.336695	-2.150746
1	3.047268	-2.976272	0.229246
16	2.377240	-0.432174	-1.337398
1	3.589252	-0.074460	0.429278
8	4.057048	0.245929	1.260430
8	-4.660230	0.779369	0.410266
7	5.306606	-0.343728	1.271464
7	-5.537002	-0.075924	0.794549
8	5.570202	-1.107016	0.363285
8	6.000668	-0.024665	2.203111
8	-6.693583	0.314780	1.030724
8	-5.206926	-1.274362	0.921195
6	0.670265	1.824166	-1.384525
1	1.126520	2.014532	-2.364046
1	-0.392293	2.066155	-1.472218
6	1.314677	2.749542	-0.334670
1	2.379850	2.510222	-0.228514
1	0.854194	2.550714	0.639299
6	1.162655	4.234306	-0.681937
1	1.615485	4.424967	-1.663231
1	0.097260	4.470894	-0.785564
6	1.792957	5.162558	0.360597
1	2.865542	4.969763	0.465980
1	1.668294	6.214429	0.086389
1	1.334140	5.018745	1.343643
39			
Bu-NO3 RC=2.0			
6	0.719880	0.512253	-1.066617
6	-0.146354	-0.385275	-0.620964
6	0.349624	-1.816617	-0.395344
6	1.564301	-2.010969	-1.345214
6	0.675981	-2.023478	1.091694
1	-0.213491	-1.818768	1.691055
1	0.977752	-3.057611	1.269360
1	1.471133	-1.352207	1.425140
6	2.483546	-3.186281	-1.035453
1	3.236594	-3.303279	-1.818883
1	1.889236	-4.103179	-0.997151
8	-0.591456	-2.804711	-0.821581
1	-1.469186	-2.550198	-0.499559
53	-2.181070	0.072486	-0.100560
1	1.131709	-2.141654	-2.338743
1	3.007490	-3.066317	-0.086106
16	2.465120	-0.396893	-1.423814
1	3.567834	-0.147587	0.410518
8	4.008800	0.178789	1.257172
8	-4.650484	0.759677	0.519041
7	5.118722	-0.612167	1.470913
7	-5.516754	-0.129992	0.853209
8	5.317558	-1.518941	0.685955
8	5.773638	-0.305061	2.435128
8	-6.671061	0.235841	1.131035
8	-5.175929	-1.330308	0.889446
6	0.659836	1.974843	-1.336566
1	1.012031	2.168076	-2.357330
1	-0.393256	2.271547	-1.298999
6	1.469141	2.831778	-0.345944

S32

1	2.522660	2.528801	-0.370137
1	1.112943	2.630205	0.670201
6	1.365874	4.331864	-0.641264
1	1.712994	4.523960	-1.664386
1	0.311731	4.631986	-0.614955
6	2.166787	5.192911	0.339978
1	3.230782	4.936448	0.314677
1	2.074201	6.257454	0.104840
1	1.817620	5.047495	1.366896

39

Bu-NO3 RC=2.2

6	0.651963	0.628617	-1.054949
6	-0.158868	-0.317281	-0.644622
6	0.351337	-1.751229	-0.461530
6	1.552107	-1.942116	-1.433167
6	0.695179	-1.982828	1.017944
1	-0.187230	-1.791721	1.632299
1	1.001196	-3.019202	1.172309
1	1.492511	-1.315630	1.352324
6	2.404311	-3.182883	-1.179252
1	3.131002	-3.318075	-1.984187
1	1.757244	-4.063736	-1.153557
8	-0.598496	-2.728046	-0.892836
1	-1.465030	-2.499671	-0.524958
53	-2.212704	0.105146	-0.096743
1	1.102893	-2.013879	-2.425218
1	2.957076	-3.121098	-0.240631
16	2.556300	-0.393624	-1.465467
1	3.596762	-0.219487	0.383187
8	4.031225	0.097449	1.241690
8	-4.654186	0.722932	0.545709
7	5.051749	-0.777991	1.540184
7	-5.500770	-0.191633	0.876262
8	5.201702	-1.735383	0.805795
8	5.690727	-0.487315	2.521297
8	-6.657146	0.150946	1.167852
8	-5.135081	-1.383069	0.893226
6	0.652553	2.087150	-1.297302
1	0.981517	2.283528	-2.324520
1	-0.390058	2.419550	-1.226126
6	1.519463	2.892582	-0.313519
1	2.556214	2.542298	-0.371177
1	1.180462	2.689253	0.707938
6	1.472787	4.399954	-0.584778
1	1.801984	4.592806	-1.613616
1	0.433862	4.745624	-0.526559
6	2.335571	5.209745	0.387580
1	3.386067	4.907365	0.330447
1	2.283845	6.280803	0.170327
1	2.006982	5.063505	1.421141

39

Bu-NO3 RC=2.4

6	0.578558	0.741652	-1.039235
6	-0.170220	-0.250728	-0.665082
6	0.356418	-1.683897	-0.508346
6	1.547758	-1.873163	-1.495377
6	0.714340	-1.922164	0.966599
1	-0.163688	-1.744127	1.591381
1	1.031189	-2.956753	1.109281
1	1.508964	-1.250330	1.296331
6	2.333735	-3.168319	-1.286939
1	3.039093	-3.317799	-2.107870
1	1.641620	-4.014436	-1.271794
8	-0.598101	-2.655833	-0.937441
1	-1.451425	-2.458088	-0.524671
53	-2.251246	0.136379	-0.100348
1	1.088041	-1.895069	-2.485082
1	2.905879	-3.158149	-0.357888
16	2.644079	-0.392166	-1.495389



### S33

1	3.643975	-0.288433	0.343958
8	4.083441	0.015667	1.211413
8	-4.662953	0.672291	0.547176
7	5.018782	-0.925718	1.568944
7	-5.479680	-0.269319	0.894315
8	5.110740	-1.920352	0.875197
8	5.654918	-0.651946	2.558394
8	-6.640281	0.045520	1.191828
8	-5.076831	-1.445971	0.917835
6	0.643659	2.192884	-1.261242
1	0.978141	2.389384	-2.285968
1	-0.388593	2.561135	-1.186758
6	1.537259	2.950002	-0.263544
1	2.556573	2.554348	-0.324439
1	1.185976	2.747740	0.753780
6	1.552793	4.460816	-0.517865
1	1.893448	4.651576	-1.543315
1	0.529143	4.849634	-0.458418
6	2.445804	5.222138	0.466274
1	3.482561	4.876166	0.408209
1	2.439839	6.296801	0.261245
1	2.108211	5.077878	1.497205

39

Bu-NO3 RC=2.6

6	0.499878	0.856910	-1.021071
6	-0.177293	-0.182270	-0.685867
6	0.365722	-1.613649	-0.551240
6	1.551718	-1.797250	-1.549457
6	0.733572	-1.856338	0.920226
1	-0.142929	-1.695968	1.552236
1	1.066406	-2.887181	1.051984
1	1.521108	-1.176057	1.247969
6	2.274024	-3.138408	-1.386909
1	2.964171	-3.292335	-2.219539
1	1.544218	-3.952291	-1.388697
8	-0.591653	-2.581331	-0.980339
1	-1.429926	-2.417404	-0.525126
53	-2.291777	0.168323	-0.106171
1	1.087005	-1.769380	-2.536913
1	2.856841	-3.180221	-0.465330
16	2.730531	-0.383877	-1.515678
1	3.692486	-0.356955	0.303919
8	4.141000	-0.073821	1.182916
8	-4.671507	0.610734	0.544058
7	4.993250	-1.070873	1.581223
7	-5.449983	-0.362994	0.910686
8	5.021779	-2.090525	0.918214
8	5.633828	-0.820149	2.575879
8	-6.615106	-0.082930	1.215488
8	-5.001894	-1.519948	0.941108
6	0.629148	2.298521	-1.225069
1	0.985640	2.491067	-2.242618
1	-0.390945	2.705509	-1.164521
6	1.533426	3.008841	-0.202434
1	2.532957	2.565467	-0.248206
1	1.152065	2.815120	0.805541
6	1.619610	4.518831	-0.446416
1	1.990903	4.700319	-1.462801
1	0.613158	4.952900	-0.406083
6	2.524185	5.233363	0.561938
1	3.545081	4.841043	0.523639
1	2.570963	6.308307	0.363911
1	2.158102	5.098494	1.584389

39

Bu-NO3 RC=2.8

6	0.414537	0.976888	-0.993368
6	-0.176833	-0.110913	-0.701717
6	0.382344	-1.539594	-0.594850
6	1.564510	-1.708342	-1.604454

S34

6	0.760815	-1.793852	0.871484
1	-0.114259	-1.657721	1.511488
1	1.113314	-2.820045	0.986179
1	1.539268	-1.104750	1.201018
6	2.228416	-3.087496	-1.497916
1	2.908126	-3.232420	-2.340392
1	1.468083	-3.872330	-1.525713
8	-0.576999	-2.501601	-1.029143
1	-1.399149	-2.373882	-0.535555
53	-2.329777	0.200038	-0.102592
1	1.097326	-1.625712	-2.587980
1	2.816068	-3.185773	-0.583694
16	2.815399	-0.360263	-1.529920
1	3.741935	-0.423266	0.264297
8	4.202748	-0.171653	1.157322
8	-4.675439	0.540290	0.552494
7	4.964051	-1.223607	1.583814
7	-5.415047	-0.473149	0.913606
8	4.918057	-2.257570	0.943189
8	5.613735	-1.007837	2.582890
8	-6.585158	-0.235359	1.225109
8	-4.921262	-1.608482	0.928577
6	0.597756	2.408840	-1.178686
1	0.973666	2.596649	-2.189976
1	-0.407828	2.853725	-1.129561
6	1.513671	3.073640	-0.134941
1	2.491215	2.583890	-0.168415
1	1.105675	2.891955	0.864735
6	1.669654	4.579255	-0.370296
1	2.069595	4.747958	-1.377876
1	0.682678	5.057581	-0.348133
6	2.584388	5.248692	0.659604
1	3.586861	4.810565	0.640235
1	2.683611	6.321044	0.467091
1	2.191577	5.126988	1.673771

39

Bu-NO3 RC=3.0

6	0.319140	1.092726	-0.968603
6	-0.162066	-0.045117	-0.720273
6	0.416859	-1.466247	-0.639361
6	1.600892	-1.609918	-1.655418
6	0.802588	-1.735062	0.821905
1	-0.073495	-1.631171	1.466916
1	1.180855	-2.753949	0.916615
1	1.566718	-1.034102	1.158806
6	2.218146	-3.016026	-1.609426
1	2.896255	-3.138792	-2.456452
1	1.436877	-3.777702	-1.673240
8	-0.538744	-2.426586	-1.085111
1	-1.346713	-2.337437	-0.561508
53	-2.360514	0.219524	-0.095182
1	1.136761	-1.472164	-2.634529
1	2.802388	-3.170515	-0.700827
16	2.906783	-0.317072	-1.531253
1	3.794084	-0.470088	0.233317
8	4.266627	-0.256635	1.142963
8	-4.669254	0.443892	0.567930
7	4.944449	-1.353925	1.581527
7	-5.362235	-0.616416	0.911445
8	4.824692	-2.391153	0.954112
8	5.607596	-1.178744	2.581926
8	-6.536621	-0.431388	1.231833
8	-4.816894	-1.724667	0.898142
6	0.528787	2.518917	-1.138355
1	0.932252	2.701817	-2.140060
1	-0.466509	2.987750	-1.112503
6	1.436774	3.154630	-0.068355
1	2.398767	2.634669	-0.080497
1	0.997314	2.983095	0.919694
6	1.641635	4.655289	-0.296770

S35

1	2.075525	4.813130	-1.291882
1	0.668508	5.162059	-0.302175
6	2.545338	5.296727	0.760332
1	3.534382	4.829045	0.769055
1	2.681644	6.365759	0.572222
1	2.119821	5.186068	1.762537

39

Bu-NO3 RC=3.2

6	0.203546	1.194339	-0.956697
6	-0.115700	0.005489	-0.750526
6	0.489131	-1.398668	-0.694721
6	1.687752	-1.494471	-1.704464
6	0.869950	-1.692813	0.762322
1	-0.014211	-1.638239	1.402726
1	1.285002	-2.699175	0.831168
1	1.607361	-0.975589	1.123017
6	2.285838	-2.910671	-1.721316
1	2.975966	-2.992206	-2.563429
1	1.500844	-3.662573	-1.835424
8	-0.449843	-2.362415	-1.171179
1	-1.247858	-2.323361	-0.627620
53	-2.375729	0.209418	-0.084613
1	1.234907	-1.305109	-2.680576
1	2.857383	-3.115459	-0.814648
16	3.015478	-0.229389	-1.509905
1	3.845367	-0.470610	0.220918
8	4.318311	-0.302004	1.157094
8	-4.638280	0.291644	0.593917
7	4.939292	-1.428856	1.587934
7	-5.269833	-0.824933	0.907193
8	4.769217	-2.459125	0.958115
8	5.613016	-1.295150	2.590276
8	-6.445773	-0.708530	1.242170
8	-4.663231	-1.895770	0.849220
6	0.385552	2.624389	-1.115668
1	0.834134	2.807040	-2.098594
1	-0.612684	3.083878	-1.139994
6	1.241117	3.267651	-0.006591
1	2.204565	2.751305	0.025743
1	0.756786	3.097940	0.960610
6	1.449287	4.768156	-0.232182
1	1.930079	4.923211	-1.205840
1	0.475020	5.270127	-0.286922
6	2.298191	5.418772	0.863965
1	3.287650	4.955739	0.922026
1	2.438595	6.487470	0.677132
1	1.825535	5.310969	1.845170

39

Bu-NO3 RC=3.4

6	-0.239491	0.794850	-0.886126
6	0.692084	-0.169685	-0.931334
6	0.760981	-1.665029	-0.575612
6	2.007365	-2.106197	-1.374324
6	0.891518	-1.837361	0.945573
1	-0.000909	-1.445741	1.436938
1	0.982515	-2.897943	1.190317
1	1.757427	-1.299797	1.337045
6	2.866674	-3.235758	-0.832995
1	3.698015	-3.440426	-1.512757
1	2.266303	-4.147404	-0.751016
8	-0.320621	-2.440193	-1.073487
1	-1.136628	-2.214015	-0.602006
53	-2.229647	0.273664	-0.158334
1	1.653862	-2.356694	-2.375267
1	3.287548	-3.005351	0.147085
16	2.853807	-0.460782	-1.530247
1	3.830705	-0.053315	0.311334
8	4.193129	0.327626	1.177083
8	-4.622723	-0.174630	0.672218

S36

7	5.395048	-0.293758	1.433673
7	-4.958928	-1.382377	0.983557
8	5.751195	-1.166277	0.665417
8	5.966565	0.107295	2.417815
8	-6.112342	-1.584975	1.387171
8	-4.120446	-2.297305	0.869635
6	-0.010989	2.229045	-1.292811
1	0.926741	2.282538	-1.857392
1	-0.815719	2.535291	-1.971058
6	0.048152	3.206173	-0.105849
1	0.864211	2.905375	0.561245
1	-0.875842	3.125468	0.476005
6	0.251298	4.659963	-0.546408
1	1.171952	4.736254	-1.138437
1	-0.567519	4.951384	-1.215787
6	0.319895	5.638285	0.630319
1	1.149355	5.391296	1.300575
1	0.463521	6.667678	0.287780
1	-0.600988	5.608592	1.221033

39

Bu-NO3 RC=3.6

6	-0.294583	0.842419	-0.913269
6	0.653162	-0.072385	-0.956166
6	0.913909	-1.548368	-0.646222
6	2.144826	-1.895878	-1.505379
6	1.123174	-1.718647	0.867308
1	0.223048	-1.407550	1.401267
1	1.314489	-2.769291	1.093859
1	1.957121	-1.112549	1.223881
6	2.992853	-3.081383	-1.069838
1	3.783095	-3.264264	-1.802843
1	2.371334	-3.980856	-1.010405
8	-0.133437	-2.399735	-1.099330
1	-0.937314	-2.242365	-0.582441
53	-2.268028	0.168390	-0.158253
1	1.758726	-2.075757	-2.509977
1	3.471577	-2.915467	-0.103520
16	3.055759	-0.282499	-1.598660
1	3.952876	0.083944	0.246914
8	4.317397	0.499566	1.105204
8	-4.585488	-0.342171	0.657050
7	5.339265	-0.293023	1.565701
7	-4.880444	-1.556097	1.014128
8	5.568002	-1.325762	0.964690
8	5.905526	0.133038	2.544369
8	-6.029498	-1.774298	1.412951
8	-4.009930	-2.438922	0.942796
6	-0.177151	2.296430	-1.292522
1	0.740585	2.421577	-1.876614
1	-1.019003	2.557669	-1.943123
6	-0.153460	3.245757	-0.082732
1	0.698802	2.985353	0.554964
1	-1.054407	3.089747	0.519566
6	-0.059805	4.719270	-0.493878
1	0.837757	4.870082	-1.106416
1	-0.913791	4.969833	-1.135280
6	-0.025320	5.673141	0.704161
1	0.836504	5.467643	1.346912
1	0.040086	6.717135	0.382819
1	-0.926087	5.568419	1.316964

39

Bu-NO3 RC=3.8

6	-0.359269	0.900678	-0.917713
6	0.589014	0.022278	-0.942252
6	1.044632	-1.404527	-0.683824
6	2.263883	-1.648085	-1.593368
6	1.320333	-1.571812	0.819773
1	0.412829	-1.359613	1.389424
1	1.623662	-2.600424	1.020973

S37

1	2.101949	-0.889597	1.154176
6	3.089160	-2.888809	-1.275236
1	3.848048	-3.030704	-2.049130
1	2.446851	-3.775639	-1.258772
8	0.050738	-2.338228	-1.110598
1	-0.740431	-2.255523	-0.559192
53	-2.322661	0.060701	-0.151865
1	1.850855	-1.745171	-2.599192
1	3.608405	-2.803210	-0.319381
16	3.247870	-0.075739	-1.607025
1	4.103763	0.174013	0.218946
8	4.480266	0.555770	1.101721
8	-4.566462	-0.515162	0.617869
7	5.400723	-0.318961	1.609282
7	-4.820518	-1.740938	1.000026
8	5.553358	-1.381883	1.035733
8	5.972349	0.066990	2.604131
8	-5.968317	-1.982594	1.377321
8	-3.916640	-2.584806	0.966649
6	-0.362774	2.364270	-1.265678
1	0.529674	2.565112	-1.866569
1	-1.237590	2.573870	-1.889943
6	-0.377139	3.283036	-0.032784
1	0.507640	3.069736	0.576943
1	-1.249493	3.048769	0.585981
6	-0.399043	4.768128	-0.411110
1	0.469774	4.995879	-1.040788
1	-1.284830	4.971441	-1.025515
6	-0.401258	5.694511	0.808711
1	0.489251	5.536472	1.425111
1	-0.417826	6.747285	0.510978
1	-1.276403	5.512553	1.440302
39			
Bu-NO3 RC=4.0			
6	-0.423876	0.994293	-0.918964
6	0.517750	0.142084	-0.925167
6	1.162463	-1.208764	-0.736182
6	2.377633	-1.323199	-1.685793
6	1.492799	-1.394357	0.753755
1	0.580913	-1.319684	1.351396
1	1.929650	-2.381744	0.907442
1	2.192018	-0.631040	1.093515
6	3.173584	-2.615240	-1.517597
1	3.910067	-2.685124	-2.322174
1	2.513024	-3.486593	-1.575116
8	0.245476	-2.223521	-1.171712
1	-0.529335	-2.235012	-0.593015
53	-2.364945	-0.059549	-0.143623
1	1.945243	-1.309501	-2.688569
1	3.720881	-2.636417	-0.573877
16	3.439741	0.195094	-1.577554
1	4.255034	0.262627	0.216822
8	4.652602	0.572482	1.137554
8	-4.519463	-0.731407	0.575293
7	5.468473	-0.393626	1.640457
7	-4.712899	-1.978657	0.964800
8	5.526165	-1.460426	1.054042
8	6.062331	-0.086349	2.652873
8	-5.852414	-2.264757	1.321941
8	-3.766813	-2.767426	0.950065
6	-0.581735	2.454067	-1.217309
1	0.269982	2.753133	-1.836000
1	-1.490568	2.598088	-1.809772
6	-0.640899	3.328193	0.046422
1	0.278263	3.177664	0.622515
1	-1.469017	2.995506	0.680632
6	-0.809301	4.815544	-0.282632
1	0.016280	5.140904	-0.927210
1	-1.727838	4.955333	-0.865888
6	-0.859266	5.699741	0.967034

S38

1	0.059865	5.605160	1.553539
1	-0.979985	6.755003	0.704636
1	-1.695269	5.419353	1.615379

39

Bu-NO3 RC=4.2

6	-0.518548	1.196018	-0.916947
6	0.410382	0.364443	-0.919065
6	1.263204	-0.865996	-0.871001
6	2.503722	-0.716943	-1.812348
6	1.620714	-1.178001	0.589525
1	0.712551	-1.347701	1.174348
1	2.235751	-2.077219	0.626999
1	2.172390	-0.349060	1.031215
6	3.284097	-2.029172	-1.937271
1	4.038840	-1.901325	-2.716949
1	2.629373	-2.861211	-2.212101
8	0.490548	-1.940216	-1.442522
1	-0.260849	-2.133575	-0.866805
53	-2.341202	-0.231118	-0.086882
1	2.079270	-0.478503	-2.790551
1	3.813029	-2.270753	-1.014214
16	3.625544	0.702557	-1.389162
1	4.364285	0.378101	0.307986
8	4.798411	0.494657	1.294729
8	-4.327937	-1.085026	0.636300
7	5.459184	-0.617757	1.677116
7	-4.441628	-2.405776	0.821167
8	5.339077	-1.628210	1.000476
8	6.120583	-0.509585	2.693578
8	-5.542970	-2.787227	1.189301
8	-3.468590	-3.122604	0.617821
6	-0.934803	2.607174	-1.121932
1	-0.189227	3.064565	-1.780632
1	-1.894618	2.629728	-1.646718
6	-1.033660	3.408640	0.187856
1	-0.063454	3.375910	0.693951
1	-1.754822	2.925360	0.854945
6	-1.447409	4.864278	-0.052638
1	-0.727293	5.339268	-0.729882
1	-2.415197	4.885625	-0.568808
6	-1.541768	5.676875	1.242168
1	-0.580071	5.699765	1.763792
1	-1.837634	6.711021	1.042925
1	-2.278793	5.244908	1.926294

39

Bu-NO3 RC=4.4

6	-0.743513	1.368376	-0.784400
6	0.329814	0.770549	-0.754734
6	1.616481	0.017169	-0.861492
6	2.765216	0.963698	-1.420512
6	1.989690	-0.651965	0.464719
1	1.231874	-1.393687	0.735238
1	2.965352	-1.137830	0.377592
1	2.047181	0.086752	1.263677
6	3.848394	0.156594	-2.150675
1	4.590319	0.856925	-2.539835
1	3.423478	-0.411393	-2.978940
8	1.400621	-0.970600	-1.888143
1	1.020782	-1.752819	-1.472758
53	-1.896277	-0.918316	-0.206997
1	2.295514	1.649023	-2.130904
1	4.354765	-0.531167	-1.469588
16	3.552890	2.096662	-0.175701
1	4.320007	1.155058	0.477158
8	5.421137	0.130409	1.572323
8	-3.194841	-2.636725	0.191962
7	5.767256	-1.065378	1.310637
7	-4.510190	-2.415963	0.448877
8	5.139518	-1.706558	0.423929

S39

8	6.710348	-1.586980	1.928462
8	-5.154754	-3.425834	0.654222
8	-4.927694	-1.269063	0.452564
6	-1.759989	2.428492	-0.867387
1	-1.307783	3.261249	-1.419146
1	-2.605932	2.075490	-1.465647
6	-2.257008	2.922786	0.504263
1	-1.398236	3.269364	1.088304
1	-2.692397	2.081448	1.051904
6	-3.291134	4.045634	0.375253
1	-2.853524	4.881762	-0.184288
1	-4.140405	3.688084	-0.219425
6	-3.794324	4.547243	1.731848
1	-2.971635	4.938779	2.338095
1	-4.530145	5.347437	1.611667
1	-4.268682	3.740404	2.298479

39

Bu-NO3 RC=4.6

6	-0.816181	1.382368	-0.730449
6	0.289919	0.850934	-0.620614
6	1.641684	0.223707	-0.741042
6	2.751677	1.369192	-0.913000
6	1.959523	-0.744418	0.397477
1	1.250966	-1.573042	0.376385
1	2.972438	-1.131464	0.260441
1	1.903658	-0.235977	1.358764
6	3.860397	0.933250	-1.884419
1	4.596926	1.736030	-1.947534
1	3.479583	0.745271	-2.892969
8	1.574127	-0.595273	-1.924423
1	1.455144	-0.025835	-2.692372
53	-1.882076	-0.985865	-0.117839
1	2.247291	2.250614	-1.320954
1	4.361922	0.031769	-1.526263
16	3.524621	2.020739	0.651544
1	4.443330	1.006506	0.859149
8	5.830784	-0.057717	1.379483
8	-3.150152	-2.691458	0.345451
7	6.035298	-1.179049	0.812124
7	-4.501915	-2.530530	0.318414
8	5.222477	-1.579936	-0.063407
8	7.026977	-1.858396	1.125280
8	-5.124706	-3.536491	0.594269
8	-4.963489	-1.438548	0.032681
6	-1.919558	2.336898	-0.913432
1	-1.528510	3.175063	-1.503096
1	-2.708061	1.869434	-1.511429
6	-2.510666	2.865837	0.407538
1	-1.710737	3.329922	0.993828
1	-2.882375	2.020977	0.994839
6	-3.642102	3.871872	0.174517
1	-3.268400	4.708167	-0.429604
1	-4.433247	3.394636	-0.416057
6	-4.235178	4.410552	1.479607
1	-3.474265	4.919974	2.079017
1	-5.040095	5.125033	1.285248
1	-4.648390	3.600402	2.087812

39

Bu-NO3 RC=4.8

6	-0.647838	1.413703	-0.561497
6	0.351803	0.766034	-0.284815
6	1.736133	0.370998	0.070961
6	2.558558	1.671656	-0.380226
6	1.803074	0.066613	1.577963
1	1.105133	-0.742971	1.800064
1	2.812698	-0.260360	1.828798
1	1.555445	0.941702	2.181680
6	3.021521	1.561816	-1.835226
1	3.441552	2.517920	-2.155324

S40

1	2.184938	1.301743	-2.491103
8	2.061828	-0.765116	-0.685640
1	3.023284	-0.992176	-0.586421
53	-1.677983	-1.012435	-0.146181
1	1.879359	2.522951	-0.294049
1	3.785012	0.790947	-1.944684
16	3.902566	2.187814	0.755532
1	4.577065	0.999817	0.817080
8	5.274053	-0.757521	1.167465
8	-2.955304	-2.800776	0.061521
7	5.499907	-1.470816	0.146878
7	-4.289801	-2.637122	0.190379
8	4.651436	-1.466998	-0.802148
8	6.524089	-2.156050	0.062706
8	-4.917726	-3.672690	0.318113
8	-4.755978	-1.506555	0.167802
6	-1.687901	2.374321	-0.936567
1	-1.175441	3.264169	-1.325617
1	-2.271087	1.964452	-1.768058
6	-2.627331	2.776552	0.215977
1	-2.029307	3.185335	1.037614
1	-3.121612	1.879944	0.600978
6	-3.679043	3.799876	-0.223479
1	-3.178541	4.692269	-0.620005
1	-4.264173	3.382025	-1.051468
6	-4.623021	4.205273	0.912176
1	-4.071000	4.654816	1.743613
1	-5.364321	4.933914	0.571937
1	-5.162627	3.337680	1.303125

39

Bu-NO3 RC=5.0

6	-0.685536	1.436926	-0.535348
6	0.352661	0.880967	-0.205757
6	1.730481	0.476311	0.178689
6	2.582219	1.785444	-0.148548
6	1.754002	0.085202	1.666822
1	1.038990	-0.722533	1.832119
1	2.751804	-0.271019	1.922580
1	1.507400	0.931632	2.311935
6	2.932600	1.864947	-1.636963
1	3.378395	2.837450	-1.856460
1	2.039511	1.735555	-2.256994
8	2.065098	-0.614950	-0.639882
1	3.035652	-0.825041	-0.606878
53	-1.655679	-1.008777	-0.109749
1	1.955699	2.641207	0.117539
1	3.646416	1.086876	-1.908958
16	4.053727	2.068498	0.927696
1	4.629738	0.829299	0.834176
8	5.331293	-0.920101	1.038457
8	-2.878259	-2.824136	0.088570
7	5.490993	-1.495206	-0.077367
7	-4.223291	-2.700365	0.174933
8	4.623295	-1.306119	-0.989664
8	6.468058	-2.220541	-0.287252
8	-4.818753	-3.754373	0.301387
8	-4.723436	-1.586645	0.119465
6	-1.757721	2.338013	-0.970744
1	-1.276105	3.230906	-1.389724
1	-2.309618	1.868042	-1.791431
6	-2.733293	2.748996	0.148029
1	-2.167801	3.219802	0.959567
1	-3.195259	1.849684	0.565583
6	-3.820793	3.704608	-0.352725
1	-3.352671	4.599299	-0.782263
1	-4.373464	3.224684	-1.169209
6	-4.800112	4.119010	0.749247
1	-4.281885	4.629014	1.567500
1	-5.566285	4.798649	0.365433
1	-5.308507	3.247093	1.171227



S41

39  
Bu-NO3 RC=5.2

6	0.515160	0.626798	-0.846780
6	0.587718	-0.593688	-0.709026
6	1.329622	-1.893347	-0.620233
6	1.458139	-2.258857	0.900709
6	0.599676	-2.979670	-1.421424
1	0.457268	-2.633726	-2.446520
1	1.215358	-3.877627	-1.432585
1	-0.372064	-3.217897	-0.985920
6	2.020683	-1.139800	1.780043
1	2.127313	-1.499957	2.804569
1	1.351097	-0.276145	1.792112
8	2.595893	-1.730735	-1.221182
1	2.977883	-0.825559	-1.070437
53	-1.869293	-0.450674	-0.175441
1	0.466027	-2.546249	1.259835
1	3.002094	-0.807076	1.433561
16	2.453386	-3.793875	1.087368
1	3.531049	-3.322226	0.427286
8	4.718490	0.799855	0.593864
8	-4.012070	-0.916062	0.388399
7	4.000913	1.436155	-0.197578
7	-4.948166	0.028480	0.235908
8	3.384111	0.810526	-1.134167
8	3.848476	2.670557	-0.107541
8	-6.083217	-0.305933	0.540359
8	-4.616586	1.131737	-0.183831
6	0.530674	2.066025	-1.041075
1	1.528470	2.261038	-1.458901
1	-0.213799	2.342379	-1.796376
6	0.346493	2.893960	0.244985
1	1.104409	2.584433	0.969766
1	-0.635844	2.682914	0.680905
6	0.492271	4.394022	-0.026169
1	1.483089	4.576852	-0.454542
1	-0.244172	4.702384	-0.779431
6	0.315435	5.240675	1.237372
1	1.064420	4.977768	1.990334
1	0.424396	6.307201	1.018759
1	-0.673854	5.090481	1.682128

39  
Bu-NO3 RC=5.4

6	0.461744	0.701663	-0.903425
6	0.642614	-0.503096	-0.702831
6	1.367481	-1.834686	-0.706366
6	1.434876	-2.422721	0.752864
6	0.646260	-2.786245	-1.673248
1	0.567104	-2.312414	-2.652784
1	1.235909	-3.697456	-1.765431
1	-0.352650	-3.043000	-1.315931
6	2.038197	-1.449759	1.765196
1	2.082180	-1.913993	2.751661
1	1.424876	-0.546730	1.840598
8	2.661253	-1.624706	-1.226668
1	3.021965	-0.723223	-1.006140
53	-1.828727	-0.378403	-0.081812
1	0.418052	-2.688445	1.054477
1	3.047390	-1.143654	1.480477
16	2.324404	-4.069080	0.808445
1	3.480173	-3.600273	0.293660
8	4.630401	0.740636	0.819427
8	-3.920482	-0.865860	0.624970
7	3.961425	1.457197	0.053117
7	-4.939490	-0.083014	0.247303
8	3.374439	0.922763	-0.956496
8	3.832553	2.682866	0.237833
8	-6.041979	-0.436567	0.636993
8	-4.706877	0.905950	-0.438661

S42

6	0.460597	2.137335	-1.140793
1	1.433465	2.321572	-1.616301
1	-0.327985	2.394330	-1.856626
6	0.353720	2.996417	0.133589
1	1.171025	2.720205	0.804519
1	-0.590562	2.779524	0.644371
6	0.447886	4.491345	-0.184511
1	1.398112	4.682809	-0.694278
1	-0.351266	4.769723	-0.883785
6	0.358905	5.365275	1.069688
1	1.171187	5.131285	1.763822
1	0.429741	6.428034	0.819058
1	-0.588360	5.209253	1.596444

37

Ph-NO3 1ec

6	4.057764	4.052773	0.468290
6	3.484185	3.913152	-0.795385
6	2.399315	3.063656	-0.981526
6	1.871047	2.344839	0.104056
6	2.455373	2.488833	1.373770
6	3.541071	3.338371	1.549590
1	4.906640	4.712436	0.609382
1	3.884894	4.464177	-1.638754
1	1.953157	2.946029	-1.961527
1	2.054784	1.925910	2.207698
1	3.987566	3.440328	2.532127
6	0.738343	1.492800	-0.080384
6	-0.317149	0.891714	-0.220006
6	-1.734361	0.462763	-0.387499
6	-2.563975	1.790275	-0.089346
6	-1.935955	-0.070290	-1.817624
1	-1.233586	-0.886013	-1.996602
1	-2.951602	-0.454333	-1.910509
1	-1.788403	0.712700	-2.565371
6	-2.697170	2.040103	1.415257
1	-3.135350	3.025707	1.585345
1	-1.719726	1.998820	1.906709
8	-1.948403	-0.545522	0.567306
1	-2.912397	-0.747990	0.698097
53	1.585738	-1.159408	-0.297972
1	-2.006674	2.614858	-0.541829
1	-3.340032	1.290233	1.877153
16	-4.190751	1.928452	-0.958833
1	-4.709795	0.699482	-0.648332
8	-5.413313	-1.059524	-0.567789
8	2.685441	-3.007280	-0.551229
7	-5.395419	-1.500355	0.617990
7	3.822355	-3.207811	0.177143
8	-4.412910	-1.192478	1.367001
8	-6.310221	-2.208864	1.049606
8	4.366393	-4.271188	-0.047578
8	4.187883	-2.345860	0.955078

37

Ph-NO3 1r

6	0.711173	4.860979	-0.078118
6	0.133516	4.011939	0.864388
6	0.185818	2.631379	0.694597
6	0.814278	2.072046	-0.427666
6	1.404407	2.936925	-1.363117
6	1.347604	4.317095	-1.193002
1	0.666331	5.936401	0.055161
1	-0.361788	4.423185	1.736957
1	-0.264355	1.980398	1.432200
1	1.898710	2.520366	-2.232996
1	1.799069	4.968046	-1.934037
6	0.875920	0.608632	-0.615943
6	-0.057555	-0.343011	-0.467244
6	0.433392	-1.787225	-0.642632
6	1.687736	-1.692712	-1.549367

S43

6	0.701770	-2.408885	0.737380
1	-0.214160	-2.381471	1.330896
1	1.006037	-3.451861	0.626356
1	1.476956	-1.863233	1.282070
6	2.663361	-2.860553	-1.512230
1	3.468085	-2.717397	-2.237752
1	2.130151	-3.778272	-1.774414
8	-0.473561	-2.612794	-1.372694
1	-1.370908	-2.447831	-1.043816
53	-2.123213	-0.080661	0.017130
1	1.303929	-1.569004	-2.564072
1	3.118555	-2.991651	-0.529151
16	2.480246	-0.072748	-1.137015
1	3.633506	-0.301143	0.703882
8	4.060435	-0.288392	1.612770
8	-4.668395	0.298008	0.635596
7	5.319359	-0.839799	1.470233
7	-5.483623	-0.694769	0.670054
8	5.633004	-1.232963	0.363808
8	5.969363	-0.868002	2.484048
8	-6.667042	-0.486632	0.986532
8	-5.066610	-1.837376	0.386038

37

Ph-NO3 RSC=1.8

6	0.707506	4.849898	-0.085397
6	0.141122	4.000906	0.863968
6	0.196097	2.620182	0.696139
6	0.815970	2.060777	-0.430631
6	1.394919	2.925519	-1.373017
6	1.335315	4.305908	-1.205074
1	0.660424	5.925432	0.046201
1	-0.347580	4.412326	1.740168
1	-0.245403	1.969069	1.438902
1	1.882356	2.508974	-2.246809
1	1.777701	4.956864	-1.951563
6	0.881223	0.595896	-0.616498
6	-0.058351	-0.350788	-0.464161
6	0.429369	-1.796443	-0.635510
6	1.686016	-1.703897	-1.539026
6	0.693950	-2.416309	0.746009
1	-0.223098	-2.386168	1.337646
1	0.996719	-3.460017	0.637533
1	1.469112	-1.871039	1.291258
6	2.666273	-2.867301	-1.493544
1	3.474426	-2.722730	-2.214968
1	2.138443	-3.787997	-1.756227
8	-0.477305	-2.621775	-1.366243
1	-1.375325	-2.452412	-1.041433
53	-2.122497	-0.080818	0.017577
1	1.305256	-1.585495	-2.555549
1	3.116312	-2.994188	-0.507527
16	2.469318	-0.077872	-1.130296
1	3.635520	-0.298478	0.705939
8	4.066711	-0.286282	1.612534
8	-4.669269	0.308051	0.633182
7	5.332595	-0.819083	1.459184
7	-5.487806	-0.681692	0.669120
8	5.645933	-1.198650	0.347995
8	5.987913	-0.846553	2.469528
8	-6.671152	-0.468887	0.983160
8	-5.074280	-1.826590	0.388833

37

Ph-NO3 RSC=2.0

6	0.718425	4.961749	0.000746
6	0.064989	4.107669	0.887522
6	0.101625	2.729713	0.695739
6	0.790325	2.178243	-0.396603
6	1.455392	3.048422	-1.276032
6	1.415047	4.425242	-1.081692

S44

1	0.687104	6.035152	0.152705
1	-0.476621	4.512736	1.735114
1	-0.408089	2.075151	1.389863
1	1.998556	2.635153	-2.117507
1	1.927925	5.080195	-1.777827
6	0.825044	0.728954	-0.610750
6	-0.044930	-0.271377	-0.498760
6	0.482813	-1.698718	-0.712011
6	1.715428	-1.578673	-1.647787
6	0.789084	-2.334634	0.653758
1	-0.117722	-2.342490	1.261864
1	1.119129	-3.366701	0.519513
1	1.556687	-1.776765	1.195465
6	2.651484	-2.780965	-1.689338
1	3.419633	-2.644960	-2.454821
1	2.073703	-3.673501	-1.943564
8	-0.422694	-2.530845	-1.435916
1	-1.312593	-2.411922	-1.069639
53	-2.124524	-0.085037	0.011757
1	1.303315	-1.406366	-2.643865
1	3.157052	-2.947719	-0.737007
16	2.584845	-0.012627	-1.205020
1	3.637974	-0.295418	0.668541
8	4.040175	-0.251186	1.590335
8	-4.649807	0.196415	0.656291
7	5.175811	-1.034597	1.574425
7	-5.434485	-0.823680	0.679218
8	5.434123	-1.622039	0.541719
8	5.789616	-1.046734	2.611451
8	-6.619377	-0.655681	1.009699
8	-4.984713	-1.946102	0.370687

37

Ph-NO3 RSC=2.2

6	0.723970	5.035962	0.059716
6	0.039142	4.185937	0.926435
6	0.055912	2.809473	0.723259
6	0.756072	2.258064	-0.363656
6	1.452358	3.123592	-1.223575
6	1.431869	4.497951	-1.015379
1	0.709409	6.108178	0.222049
1	-0.511374	4.592915	1.767318
1	-0.480193	2.155938	1.398395
1	2.007952	2.703718	-2.053209
1	1.970961	5.150833	-1.693282
6	0.754528	0.821739	-0.589508
6	-0.046823	-0.221026	-0.512584
6	0.513160	-1.635662	-0.735356
6	1.733965	-1.510397	-1.690212
6	0.841395	-2.261541	0.629944
1	-0.060168	-2.286431	1.245611
1	1.190216	-3.286999	0.494435
1	1.601762	-1.687080	1.163152
6	2.619711	-2.750944	-1.779475
1	3.363332	-2.632886	-2.571512
1	1.999048	-3.617644	-2.021518
8	-0.388798	-2.481638	-1.446887
1	-1.269946	-2.402028	-1.050916
53	-2.146357	-0.085372	0.003581
1	1.304559	-1.306519	-2.672799
1	3.154807	-2.945708	-0.848809
16	2.686885	0.001062	-1.247143
1	3.682622	-0.317159	0.623138
8	4.080359	-0.261021	1.550420
8	-4.643882	0.124931	0.642920
7	5.127334	-1.154510	1.605187
7	-5.402630	-0.918329	0.676270
8	5.335652	-1.834730	0.618916
8	5.727012	-1.160302	2.651602
8	-6.589655	-0.773779	1.004765
8	-4.923278	-2.029764	0.380088

S45

37  
Ph-NO3 RSC=2.4

6	0.706927	5.087390	0.114911
6	0.133204	4.225929	1.048526
6	0.134427	2.851955	0.830290
6	0.703798	2.319796	-0.340205
6	1.287505	3.196169	-1.270672
6	1.285363	4.566770	-1.044130
1	0.707027	6.157704	0.289856
1	-0.317044	4.622455	1.951664
1	-0.317126	2.183742	1.552107
1	1.748131	2.783075	-2.159560
1	1.737487	5.231787	-1.771777
6	0.671439	0.896918	-0.574774
6	-0.048903	-0.187370	-0.524274
6	0.545350	-1.589251	-0.739966
6	1.755456	-1.462249	-1.713397
6	0.896245	-2.187675	0.631655
1	0.000381	-2.224670	1.255369
1	1.266989	-3.206539	0.506665
1	1.647909	-1.588521	1.148645
6	2.596043	-2.734613	-1.834226
1	3.317620	-2.634223	-2.648476
1	1.941669	-3.581033	-2.058588
8	-0.351553	-2.457622	-1.429835
1	-1.221727	-2.411889	-1.006291
53	-2.171757	-0.087279	-0.002886
1	1.309312	-1.240937	-2.684765
1	3.155424	-2.946697	-0.921715
16	2.780598	0.004523	-1.292465
1	3.742112	-0.327436	0.555615
8	4.141310	-0.256043	1.487561
8	-4.635621	0.060939	0.629584
7	5.112493	-1.221382	1.607091
7	-5.369919	-1.004079	0.677584
8	5.274473	-1.976891	0.667761
8	5.705046	-1.210576	2.659112
8	-6.558312	-0.877866	1.002377
8	-4.863311	-2.105417	0.399504

37  
Ph-NO3 RSC=2.6

6	0.778398	5.147395	0.162860
6	1.026767	4.252121	1.204304
6	0.966167	2.882906	0.977522
6	0.653118	2.390406	-0.302700
6	0.411075	3.300753	-1.347544
6	0.469077	4.668225	-1.111182
1	0.824625	6.215683	0.343800
1	1.264429	4.622793	2.195020
1	1.157404	2.181247	1.780010
1	0.176603	2.918703	-2.333358
1	0.272637	5.363000	-1.920075
6	0.575293	0.983671	-0.536126
6	-0.053665	-0.139086	-0.542856
6	0.555739	-1.521002	-0.827397
6	1.758510	-1.353500	-1.807716
6	0.919567	-2.172361	0.515594
1	0.030069	-2.242207	1.145823
1	1.297162	-3.181568	0.344230
1	1.672459	-1.589339	1.048037
6	2.546935	-2.650922	-2.018862
1	3.250647	-2.527772	-2.845174
1	1.859085	-3.463007	-2.269085
8	-0.351254	-2.357169	-1.543715
1	-1.202407	-2.366751	-1.081886
53	-2.184890	-0.080931	0.055206
1	1.301729	-1.066522	-2.757045
1	3.123361	-2.926867	-1.134334
16	2.860320	0.041226	-1.342632

S46

1	3.759726	-0.382785	0.460629
8	4.147456	-0.335519	1.409889
8	-4.600122	-0.019893	0.739526
7	5.041772	-1.362023	1.569551
7	-5.314748	-1.104256	0.746670
8	5.170836	-2.149269	0.651050
8	5.612947	-1.372810	2.635501
8	-6.500187	-1.009116	1.086288
8	-4.790241	-2.180295	0.417793

37

Ph-NO3 RSC=2.8

6	0.813506	5.222896	0.221529
6	1.078995	4.319281	1.252444
6	0.976747	2.953582	1.026933
6	0.605652	2.471615	-0.244021
6	0.344920	3.391479	-1.278676
6	0.444813	4.755500	-1.041390
1	0.893635	6.289185	0.402199
1	1.364238	4.682326	2.233293
1	1.184183	2.244553	1.818622
1	0.066153	3.017155	-2.255711
1	0.236592	5.457531	-1.840900
6	0.483378	1.077984	-0.475654
6	-0.059010	-0.075548	-0.533173
6	0.573005	-1.444328	-0.838238
6	1.772330	-1.259945	-1.823818
6	0.947065	-2.101437	0.498696
1	0.058749	-2.198319	1.127352
1	1.347517	-3.099623	0.315777
1	1.687251	-1.507695	1.036233
6	2.505986	-2.580222	-2.099403
1	3.199119	-2.446384	-2.932683
1	1.786680	-3.358815	-2.366481
8	-0.331828	-2.278623	-1.558412
1	-1.169148	-2.329298	-1.075413
53	-2.223383	-0.071849	0.062733
1	1.311480	-0.922482	-2.754699
1	3.090062	-2.907116	-1.237495
16	2.947656	0.064343	-1.335807
1	3.818065	-0.439676	0.419222
8	4.221001	-0.426405	1.372804
8	-4.605837	-0.103999	0.716680
7	5.036691	-1.511839	1.531440
7	-5.279518	-1.220413	0.715718
8	5.097953	-2.317016	0.620727
8	5.619945	-1.557434	2.591817
8	-6.468364	-1.164667	1.044283
8	-4.710658	-2.272132	0.391759

37

Ph-NO3 RSC=3.0

6	0.732533	5.312061	0.285798
6	0.998906	4.404631	1.313799
6	0.887891	3.040811	1.086337
6	0.508527	2.563702	-0.185633
6	0.245035	3.488327	-1.217151
6	0.353887	4.850500	-0.976558
1	0.820425	6.377369	0.468470
1	1.293020	4.764318	2.293193
1	1.097739	2.328119	1.873926
1	-0.040182	3.117698	-2.193643
1	0.146562	5.556051	-1.773096
6	0.379765	1.177588	-0.419521
6	-0.055039	-0.007563	-0.523571
6	0.614161	-1.355574	-0.844661
6	1.812793	-1.140687	-1.829970
6	1.000946	-2.014506	0.487202
1	0.113070	-2.150459	1.109548
1	1.438138	-2.995174	0.294257
1	1.717903	-1.401539	1.033924

S47

6	2.506916	-2.469149	-2.172523
1	3.197996	-2.310400	-3.002894
1	1.768301	-3.218100	-2.469007
8	-0.276966	-2.197711	-1.572380
1	-1.100620	-2.295592	-1.074284
53	-2.254326	-0.082540	0.066975
1	1.350633	-0.753293	-2.740856
1	3.090532	-2.847225	-1.331526
16	3.042828	0.121641	-1.310065
1	3.892584	-0.466383	0.390743
8	4.314638	-0.495999	1.345621
8	-4.603033	-0.237550	0.686714
7	5.056834	-1.630791	1.485644
7	-5.214769	-1.395005	0.677270
8	5.045824	-2.439196	0.574839
8	5.659882	-1.719661	2.533988
8	-6.406201	-1.399260	0.993062
8	-4.584697	-2.410283	0.359519

37

Ph-NO3 RSC=3.2

6	0.439051	5.424862	0.349880
6	0.761314	4.525324	1.369114
6	0.702850	3.159328	1.137684
6	0.322062	2.672196	-0.130648
6	0.001064	3.589223	-1.153396
6	0.057622	4.953525	-0.908038
1	0.486226	6.492147	0.535902
1	1.059040	4.893346	2.344254
1	0.958077	2.452435	1.916955
1	-0.286030	3.211045	-2.126433
1	-0.191811	5.653306	-1.697485
6	0.252407	1.285797	-0.370192
6	-0.034525	0.069256	-0.516782
6	0.695243	-1.239676	-0.859701
6	1.897301	-0.960363	-1.830734
6	1.096979	-1.909945	0.461275
1	0.209320	-2.113740	1.065415
1	1.594449	-2.857429	0.249724
1	1.770211	-1.271417	1.033337
6	2.579446	-2.272616	-2.256793
1	3.277066	-2.061040	-3.069560
1	1.839528	-2.996737	-2.605847
8	-0.161891	-2.095711	-1.612669
1	-0.971452	-2.258630	-1.109396
53	-2.265288	-0.138319	0.080960
1	1.436066	-0.515568	-2.715773
1	3.157191	-2.707319	-1.439556
16	3.151299	0.252340	-1.246772
1	3.984008	-0.437202	0.385589
8	4.426663	-0.523481	1.338848
8	-4.562097	-0.470996	0.683599
7	5.113768	-1.692296	1.434205
7	-5.090865	-1.673508	0.625601
8	5.035983	-2.483670	0.510538
8	5.745015	-1.834153	2.461664
8	-6.276445	-1.768766	0.940569
8	-4.390679	-2.624547	0.267664

37

Ph-NO3 RSC=3.4

6	-0.139330	5.521127	0.415187
6	0.300673	4.653457	1.417846
6	0.373542	3.289661	1.177248
6	0.008723	2.774329	-0.084057
6	-0.431645	3.658664	-1.090311
6	-0.505902	5.020702	-0.835633
1	-0.194623	6.586703	0.608564
1	0.588409	5.044705	2.386885
1	0.722267	2.607762	1.942368
1	-0.706858	3.258790	-2.058162

S48

1	-0.845694	5.695904	-1.612619
6	0.082067	1.389616	-0.335310
6	0.011135	0.155335	-0.518863
6	0.827822	-1.085809	-0.890248
6	2.034197	-0.693382	-1.823135
6	1.248413	-1.783884	0.409151
1	0.366589	-2.088773	0.978476
1	1.829565	-2.674575	0.167154
1	1.854185	-1.120787	1.026621
6	2.747811	-1.952652	-2.349006
1	3.458849	-1.651999	-3.120939
1	2.033214	-2.657837	-2.779420
8	0.032545	-1.957099	-1.695039
1	-0.755677	-2.215748	-1.199032
53	-2.246499	-0.259472	0.102130
1	1.570768	-0.188154	-2.674227
1	3.317848	-2.447041	-1.560872
16	3.263189	0.492657	-1.132760
1	4.088506	-0.305556	0.408530
8	4.552212	-0.458096	1.357737
8	-4.452632	-0.829272	0.698018
7	5.212431	-1.640372	1.386759
7	-4.868751	-2.076908	0.561304
8	5.083217	-2.399674	0.440494
8	5.879017	-1.836354	2.384582
8	-6.034508	-2.295323	0.878551
8	-4.087944	-2.928667	0.136191

37

Ph-NO3 RSC=3.6

6	0.090070	5.280695	0.057504
6	0.817811	4.578300	-0.903104
6	0.678802	3.199457	-1.021996
6	-0.194512	2.491864	-0.178684
6	-0.928407	3.209112	0.776391
6	-0.781218	4.588521	0.896396
1	0.197845	6.356228	0.147657
1	1.495105	5.105671	-1.566475
1	1.246667	2.656637	-1.767055
1	-1.615121	2.681953	1.426495
1	-1.354366	5.122454	1.646644
6	-0.315014	1.024849	-0.308207
6	0.636883	0.173682	-0.670502
6	0.856108	-1.324314	-0.923037
6	2.102439	-1.362552	-1.828823
6	1.029507	-2.043648	0.425037
1	0.123729	-1.931762	1.023618
1	1.198914	-3.107898	0.250221
1	1.865392	-1.630751	0.991353
6	2.919377	-2.645571	-1.847688
1	3.724929	-2.564961	-2.582361
1	2.280747	-3.486667	-2.136314
8	-0.188705	-1.924774	-1.677707
1	-0.995771	-1.984622	-1.145064
53	-2.281014	0.071808	0.143925
1	1.739789	-1.149719	-2.835713
1	3.375926	-2.861240	-0.880586
16	3.033985	0.148057	-1.295851
1	3.934438	-0.236779	0.567121
8	4.303026	-0.205146	1.514539
8	-4.537406	-0.814659	0.712442
7	5.320173	-1.124227	1.604893
7	-4.775235	-2.081670	0.536304
8	5.540167	-1.819846	0.631395
8	5.889973	-1.140826	2.669609
8	-5.898391	-2.499364	0.832930
8	-3.877903	-2.810935	0.084035

37

Ph-NO3 RSC=3.8

6	-0.313343	5.351187	0.162025
---	-----------	----------	----------



S49

6	0.649823	4.694130	-0.605012
6	0.615689	3.311901	-0.745282
6	-0.389502	2.555127	-0.116900
6	-1.354356	3.223834	0.647441
6	-1.312197	4.609208	0.787663
1	-0.285465	6.430299	0.268204
1	1.433033	5.260029	-1.097959
1	1.369320	2.801644	-1.332439
1	-2.138064	2.658278	1.134161
1	-2.066859	5.106651	1.387077
6	-0.390175	1.089744	-0.275676
6	0.553725	0.264415	-0.613798
6	0.988626	-1.162546	-0.919324
6	2.214477	-1.054509	-1.847226
6	1.252883	-1.893735	0.408060
1	0.343169	-1.910392	1.011838
1	1.549729	-2.922897	0.199964
1	2.035869	-1.397029	0.980926
6	3.018101	-2.335954	-2.030842
1	3.782658	-2.180218	-2.796449
1	2.362286	-3.148083	-2.361452
8	-0.003121	-1.853006	-1.678578
1	-0.789139	-2.010581	-1.136004
53	-2.323594	-0.068594	0.135312
1	1.810801	-0.748692	-2.814310
1	3.528990	-2.636034	-1.114726
16	3.216184	0.381304	-1.241227
1	4.100586	-0.126653	0.534200
8	4.496820	-0.134695	1.483966
8	-4.482881	-1.028243	0.648534
7	5.401737	-1.156851	1.577135
7	-4.659631	-2.317717	0.484557
8	5.519491	-1.901762	0.621561
8	5.995518	-1.213019	2.630001
8	-5.773270	-2.764984	0.756503
8	-3.720383	-3.008864	0.073816

37

Ph-NO3 RSC=4.0

6	-0.755516	5.404768	0.300134
6	0.453665	4.802041	-0.052140
6	0.529829	3.426575	-0.229943
6	-0.614404	2.625778	-0.054214
6	-1.823352	3.236054	0.299686
6	-1.890392	4.616849	0.474126
1	-0.810536	6.479280	0.437613
1	1.344524	5.405319	-0.189042
1	1.466619	2.952932	-0.503456
1	-2.709918	2.631947	0.439286
1	-2.835034	5.073510	0.748273
6	-0.478623	1.181510	-0.256313
6	0.429788	0.352636	-0.565326
6	1.104589	-0.942930	-0.925592
6	2.318974	-0.635681	-1.840409
6	1.455795	-1.700922	0.365288
1	0.549942	-1.901621	0.942450
1	1.922603	-2.652318	0.107936
1	2.137915	-1.116595	0.981650
6	3.105314	-1.881980	-2.242388
1	3.838606	-1.602539	-3.003154
1	2.440651	-2.643896	-2.661804
8	0.211786	-1.721255	-1.736698
1	-0.546922	-2.003532	-1.207984
53	-2.352837	-0.240523	0.141741
1	1.881068	-0.198200	-2.740250
1	3.656953	-2.303402	-1.400784
16	3.397849	0.684266	-1.108197
1	4.257576	-0.029694	0.509743
8	4.692478	-0.141511	1.460368
8	-4.382711	-1.273649	0.631557
7	5.480578	-1.249226	1.486805

## S50

7	-4.501486	-2.580901	0.433493
8	5.474834	-1.983800	0.513974
8	6.118305	-1.400644	2.508218
8	-5.597292	-3.063913	0.692146
8	-3.533267	-3.213856	0.015294

37

Ph-NO3 RSC=4.2

6	-1.540603	5.395775	0.452721
6	-0.221218	4.970844	0.285804
6	0.064027	3.628995	0.066859
6	-0.982626	2.687954	0.014978
6	-2.303669	3.117911	0.185994
6	-2.577204	4.466446	0.401364
1	-1.757662	6.444600	0.623282
1	0.592321	5.686575	0.326628
1	1.086723	3.289892	-0.063787
1	-3.111694	2.398891	0.151855
1	-3.604562	4.787950	0.531539
6	-0.614453	1.305930	-0.229106
6	0.297192	0.504039	-0.512335
6	1.225563	-0.583554	-0.934656
6	2.439760	0.026234	-1.734375
6	1.648722	-1.418189	0.281888
1	0.776289	-1.887476	0.744588
1	2.340670	-2.197001	-0.038848
1	2.142585	-0.786789	1.019515
6	3.243561	-1.073442	-2.438978
1	3.981041	-0.586356	-3.081064
1	2.604272	-1.713093	-3.053134
8	0.515413	-1.396821	-1.889695
1	-0.193225	-1.869707	-1.434563
53	-2.280102	-0.500022	0.168688
1	1.979948	0.653770	-2.501783
1	3.793641	-1.686358	-1.723862
16	3.549545	1.148692	-0.754847
1	4.381356	0.138775	0.571847
8	4.896825	-0.165625	1.484489
8	-4.109262	-1.714826	0.668427
7	5.511907	-1.353945	1.336535
7	-4.161383	-2.999784	0.277888
8	5.258991	-2.022528	0.343882
8	6.273368	-1.667498	2.234133
8	-5.199625	-3.580018	0.549181
8	-3.196586	-3.483826	-0.300051

37

Ph-NO3 RSC=4.4

6	-3.955716	4.133311	-0.244400
6	-3.144471	4.081135	0.888796
6	-2.075911	3.192983	0.944771
6	-1.804621	2.346630	-0.143653
6	-2.626867	2.403307	-1.281481
6	-3.694283	3.291944	-1.326415
1	-4.790999	4.823605	-0.283027
1	-3.345294	4.731688	1.732548
1	-1.443303	3.145126	1.822625
1	-2.424910	1.741720	-2.114709
1	-4.326109	3.325556	-2.206661
6	-0.686178	1.457728	-0.093080
6	0.365192	0.833050	-0.064335
6	1.783404	0.390618	-0.058972
6	2.618028	1.729058	-0.425738
6	2.126167	-0.226909	1.309424
1	1.543725	-1.142123	1.427009
1	3.188081	-0.476782	1.328149
1	1.902700	0.455444	2.129072
6	3.620043	1.507783	-1.562336
1	4.078316	2.465575	-1.819446
1	3.116100	1.102454	-2.440868
8	1.915834	-0.570828	-1.079301

## S51

1	2.779895	-1.045481	-0.957856
53	-1.554656	-1.160131	0.242770
1	1.898052	2.482241	-0.752574
1	4.404083	0.813050	-1.260101
16	3.424688	2.574405	1.008651
1	4.397199	1.653142	1.185244
8	5.294040	-0.584553	0.472033
8	-2.664549	-2.985804	0.620115
7	5.287491	-1.656052	-0.196568
7	-3.846787	-3.188872	-0.027838
8	4.248476	-1.959706	-0.868837
8	6.271380	-2.407611	-0.208397
8	-4.390109	-4.238052	0.258494
8	-4.251249	-2.341964	-0.804016

37

Ph-NO3 RSC=4.6

6	-3.724657	4.350333	-0.156185
6	-3.123541	4.043560	1.064876
6	-2.126577	3.077634	1.130092
6	-1.714403	2.409015	-0.036494
6	-2.325599	2.723635	-1.263444
6	-3.324221	3.687919	-1.317260
1	-4.505559	5.101122	-0.202456
1	-3.434797	4.555569	1.968286
1	-1.658916	2.829436	2.074938
1	-2.013119	2.201016	-2.158993
1	-3.793359	3.921812	-2.266053
6	-0.671945	1.440575	0.023596
6	0.279131	0.667957	0.049766
6	1.705779	0.257821	0.144377
6	2.466907	1.576312	-0.385998
6	2.003913	-0.120616	1.607076
1	1.356369	-0.955097	1.883878
1	3.044435	-0.439130	1.684944
1	1.838884	0.715797	2.287624
6	2.892347	1.432271	-1.849232
1	3.279853	2.389088	-2.206089
1	2.042786	1.135639	-2.470997
8	1.903731	-0.845235	-0.699383
1	2.859514	-1.109858	-0.687991
53	-1.627559	-1.173197	0.225173
1	1.761117	2.405257	-0.317878
1	3.668403	0.674384	-1.962911
16	3.817487	2.189551	0.689953
1	4.589102	1.064767	0.667728
8	5.325606	-0.755688	0.824584
8	-2.811634	-2.996069	0.507977
7	5.449747	-1.507216	-0.185452
7	-3.980478	-3.136988	-0.166497
8	4.481816	-1.598632	-1.006996
8	6.491661	-2.142519	-0.381355
8	-4.562642	-4.182376	0.057229
8	-4.348737	-2.243515	-0.910913

37

Ph-NO3 RSC=4.8

6	-3.874489	4.226749	-0.283529
6	-3.313439	3.959049	0.965349
6	-2.276995	3.040610	1.083921
6	-1.784915	2.380604	-0.055759
6	-2.356357	2.654823	-1.310727
6	-3.394179	3.572340	-1.418417
1	-4.686066	4.940321	-0.371781
1	-3.686728	4.464124	1.848994
1	-1.840674	2.822657	2.051019
1	-1.982522	2.138444	-2.186156
1	-3.831737	3.775195	-2.389209
6	-0.702557	1.459615	0.059160
6	0.289242	0.746613	0.136372
6	1.715908	0.345595	0.267855

S52

6	2.478275	1.691021	-0.144704
6	1.974151	-0.107610	1.715939
1	1.304658	-0.938261	1.947222
1	3.005031	-0.453069	1.799351
1	1.816187	0.703029	2.430175
6	2.705134	1.761767	-1.656923
1	3.083939	2.751359	-1.921517
1	1.772089	1.581391	-2.199829
8	1.940320	-0.703670	-0.636116
1	2.906801	-0.923067	-0.699984
53	-1.602624	-1.176774	0.247770
1	1.836509	2.522775	0.153343
1	3.430228	1.013266	-1.977925
16	3.999091	2.062692	0.814679
1	4.644537	0.868755	0.645731
8	5.371491	-0.906396	0.730886
8	-2.743068	-3.020395	0.501449
7	5.441145	-1.495623	-0.386735
7	-3.908243	-3.177319	-0.181247
8	4.475095	-1.368073	-1.205974
8	6.425875	-2.178093	-0.687153
8	-4.468981	-4.235792	0.031905
8	-4.289187	-2.284760	-0.918928

37

Ph-NO3 RSC=5.0

6	-4.047063	4.066984	-0.437122
6	-3.467079	3.917022	0.822462
6	-2.384954	3.061707	0.997241
6	-1.865887	2.347408	-0.095853
6	-2.456620	2.501966	-1.361455
6	-3.539579	3.357202	-1.525826
1	-4.893849	4.731161	-0.569302
1	-3.860701	4.464513	1.671440
1	-1.933821	2.935961	1.973944
1	-2.063030	1.942632	-2.201110
1	-3.991151	3.467310	-2.505153
6	-0.736209	1.489578	0.076828
6	0.313822	0.876796	0.206466
6	1.733426	0.454461	0.365107
6	2.549689	1.788534	0.056032
6	1.947334	-0.074005	1.795066
1	1.250359	-0.893118	1.979846
1	2.965556	-0.452836	1.882216
1	1.800260	0.709683	2.542029
6	2.687230	2.022264	-1.450733
1	3.114912	3.010858	-1.630132
1	1.712792	1.963673	-1.946272
8	1.949173	-0.553891	-0.588810
1	2.913445	-0.763149	-0.706633
53	-1.583965	-1.162627	0.291342
1	1.981074	2.612218	0.495606
1	3.340681	1.274413	-1.900856
16	4.168014	1.954922	0.932429
1	4.699414	0.726596	0.642435
8	5.399931	-1.038158	0.596323
8	-2.684393	-3.011982	0.546309
7	5.398612	-1.503013	-0.580499
7	-3.824028	-3.210748	-0.177094
8	4.423242	-1.216726	-1.347039
8	6.322752	-2.214374	-0.986782
8	-4.367580	-4.274633	0.047119
8	-4.193219	-2.346809	-0.951392

37

Ph-NO3 RSC=5.2

6	0.090620	5.088348	-0.019608
6	-1.095827	4.437088	-0.358831
6	-1.116495	3.056351	-0.518082
6	0.061042	2.314624	-0.331805
6	1.259864	2.969514	0.014198

S53

6	1.261467	4.352800	0.162334
1	0.100775	6.165845	0.104619
1	-2.009692	5.003850	-0.497103
1	-2.038490	2.548678	-0.771802
1	2.173251	2.395892	0.143820
1	2.187315	4.851986	0.424712
6	0.119651	0.895617	-0.511285
6	0.426307	-0.281177	-0.692889
6	1.286175	-1.471559	-0.977039
6	1.527406	-2.255424	0.368126
6	0.645012	-2.377507	-2.034199
1	0.509122	-1.814482	-2.958847
1	1.325278	-3.208422	-2.223864
1	-0.320392	-2.763449	-1.702423
6	1.723791	-1.388532	1.615902
1	1.934631	-2.031289	2.471916
1	0.824796	-0.807659	1.838457
8	2.458537	-0.957464	-1.557141
1	2.953865	-0.349150	-0.942625
53	-2.060849	-0.542147	0.037296
1	0.656886	-2.899386	0.519880
1	2.559074	-0.699211	1.490795
16	2.919872	-3.433770	0.163377
1	3.897367	-2.494742	0.156491
8	5.166885	-0.661968	0.550391
8	-4.038838	-1.386524	0.638968
7	4.831614	0.542770	0.507105
7	-5.149006	-0.651574	0.439574
8	3.715221	0.853248	-0.051980
8	5.533843	1.438010	0.992091
8	-6.191057	-1.196818	0.760958
8	-5.039476	0.473568	-0.029842

37

Ph-NO3 RSC=5.4

6	0.191323	5.157496	-0.267593
6	-0.938762	4.484178	-0.735769
6	-0.932340	3.099191	-0.842488
6	0.213378	2.375606	-0.469720
6	1.354276	3.052592	0.003033
6	1.331229	4.440896	0.094752
1	0.180533	6.239112	-0.185181
1	-1.827812	5.038349	-1.015013
1	-1.810638	2.572505	-1.194507
1	2.243158	2.482375	0.258582
1	2.213041	4.958576	0.454733
6	0.284975	0.953229	-0.590213
6	0.554914	-0.245862	-0.683186
6	1.290230	-1.510013	-1.061433
6	1.321914	-2.509372	0.151107
6	0.595739	-2.121743	-2.288299
1	0.567943	-1.382892	-3.090324
1	1.173093	-2.984941	-2.617437
1	-0.422390	-2.439505	-2.055140
6	1.865096	-1.898176	1.443047
1	1.812433	-2.632452	2.248833
1	1.274206	-1.025081	1.735887
8	2.581544	-1.134808	-1.472412
1	3.017704	-0.505728	-0.831090
53	-1.915555	-0.436418	0.162026
1	0.300693	-2.864354	0.312845
1	2.905127	-1.584130	1.332505
16	2.241993	-4.069499	-0.270384
1	3.429573	-3.465657	-0.482744
8	5.049419	-0.446028	1.067560
8	-3.872339	-1.174734	0.919191
7	4.559974	0.683042	0.870970
7	-5.003676	-0.544058	0.541777
8	3.578353	0.801597	0.047192
8	4.980576	1.698329	1.447814
8	-6.030963	-1.037854	0.973541

S54

8 -4.922846 0.442869 -0.175617

55

Bu-EtSO4 1ec

6	-0.725584	-0.244638	-0.692840
6	-0.130155	0.712764	-0.174274
6	-0.158724	2.117472	0.405576
6	-1.065950	2.962366	-0.540532
6	-0.708790	1.993139	1.833801
1	-0.083635	1.309690	2.415761
1	-0.692283	2.977021	2.302967
1	-1.729667	1.606833	1.811178
6	-0.430885	3.190485	-1.913870
1	-1.154388	3.664078	-2.579084
1	-0.122647	2.240736	-2.358773
8	1.125806	2.721077	0.392116
1	1.725267	2.198567	0.938436
53	1.806609	-0.647390	0.148343
1	-2.009103	2.426036	-0.632784
1	0.452453	3.827539	-1.842177
16	-1.505937	4.616739	0.184185
1	-2.695263	4.240026	0.694943
8	-3.452987	1.000369	0.102785
8	3.803100	-1.629216	0.762228
8	-4.489735	-0.572612	-1.500974
8	-5.811536	1.350430	-0.639833
8	6.202083	-2.163080	0.736903
8	5.064977	-1.521515	-1.394959
16	5.146649	-1.415611	0.060998
16	-4.709472	0.407558	-0.406674
8	5.368418	0.191866	0.413345
8	-5.178605	-0.522749	0.917210
6	6.540733	0.805705	-0.162840
1	6.488317	0.720092	-1.252278
1	7.430748	0.274883	0.190556
6	6.550871	2.256057	0.280807
1	6.592938	2.327364	1.370053
1	7.426165	2.764749	-0.134366
1	5.653691	2.773054	-0.066814
6	-6.456532	-1.163133	0.802419
1	-7.228608	-0.403680	0.641299
1	-6.450508	-1.836718	-0.062516
6	-6.700751	-1.929931	2.090677
1	-6.697631	-1.252371	2.948091
1	-7.671678	-2.434153	2.049767
1	-5.925689	-2.684514	2.246880
6	-1.452153	-1.330679	-1.301309
6	-1.751258	-2.518085	-0.363846
1	-0.932237	-1.656768	-2.209998
1	-2.418667	-0.892202	-1.614794
6	-2.587128	-3.588963	-1.071385
1	-0.811070	-2.947864	-0.001245
1	-2.296304	-2.139630	0.505457
6	-2.919992	-4.772322	-0.158428
1	-3.509315	-3.125875	-1.435440
1	-2.043461	-3.951049	-1.953545
1	-3.517358	-5.522934	-0.684542
1	-2.011967	-5.264328	0.205944
1	-3.492591	-4.443884	0.714383

55

Bu-EtSO4 1r

6	1.498681	-1.371958	-1.275955
6	0.543467	-1.716813	-0.407521
6	0.992233	-2.439783	0.864211
6	2.374297	-3.058890	0.515302
6	1.017335	-1.472807	2.055234
1	0.017367	-1.060885	2.207875
1	1.308102	-2.004295	2.963843
1	1.703616	-0.640006	1.888454

S55

6	3.310675	-3.371314	1.674564
1	4.214564	-3.871511	1.316370
1	2.807320	-4.048183	2.370203
8	0.168035	-3.568421	1.176991
1	-0.756067	-3.280769	1.154353
53	-1.508020	-1.210842	-0.613018
1	2.150494	-3.975553	-0.033435
1	3.611422	-2.474509	2.219067
16	3.138452	-1.930549	-0.743971
1	4.054335	-0.398672	0.491147
8	4.559268	0.149587	1.163102
8	-4.132148	-0.520020	-0.885973
8	4.431232	2.116941	-0.393530
8	5.096802	2.375215	2.013681
8	-6.474009	0.098506	-0.325507
8	-4.936741	-0.694173	1.463714
16	-5.088115	-0.047004	0.147547
16	4.310745	1.711080	0.997405
8	-4.527445	1.538798	0.373497
8	2.738721	1.721866	1.407708
6	-5.276005	2.319433	1.307424
1	-5.284137	1.817565	2.282271
1	-6.311872	2.410863	0.960613
6	-4.611840	3.683227	1.403545
1	-4.599173	4.174941	0.427281
1	-5.156724	4.321441	2.107340
1	-3.580214	3.585369	1.751905
6	2.005389	2.973256	1.204840
1	2.489699	3.752770	1.799348
1	2.064612	3.233769	0.146294
6	0.580658	2.727046	1.651268
1	0.544053	2.450407	2.706654
1	-0.002346	3.641797	1.514042
1	0.112091	1.935376	1.064505
6	1.393164	-0.626454	-2.574601
6	1.658117	0.886770	-2.461142
1	0.385834	-0.784472	-2.971100
1	2.093565	-1.064302	-3.295621
6	1.554459	1.603181	-3.812044
1	0.929508	1.315685	-1.764150
1	2.648837	1.065398	-2.030845
6	1.782723	3.114125	-3.706148
1	2.286810	1.171484	-4.506080
1	0.567082	1.411781	-4.248977
1	1.719432	3.597157	-4.685927
1	1.031683	3.579484	-3.059852
1	2.767993	3.335556	-3.284621

55

Bu-EtSO4 RCS=1.8

6	1.544455	-0.930587	-1.590287
6	0.993449	-1.723206	-0.665352
6	1.945313	-2.500113	0.243443
6	3.299042	-2.533308	-0.520528
6	2.023437	-1.864243	1.636673
1	1.030177	-1.859655	2.090157
1	2.688650	-2.447073	2.277315
1	2.372981	-0.831419	1.595582
6	4.563896	-2.722192	0.305896
1	5.439592	-2.802382	-0.343996
1	4.486379	-3.650921	0.877820
8	1.569766	-3.880401	0.366676
1	0.628550	-3.909178	0.588934
53	-1.082725	-1.770424	-0.246928
1	3.205367	-3.347866	-1.241083
1	4.730898	-1.898571	1.002146
16	3.343048	-0.992491	-1.555197
1	3.916695	0.526872	-0.043187
8	4.312356	1.042128	0.715096
8	-3.727263	-1.516164	0.592632
8	3.255315	3.125846	-0.205941

S56

8	4.242177	3.051577	2.101442
8	-5.409911	-0.384181	2.037183
8	-3.257757	0.748009	1.514023
16	-4.280029	-0.238693	1.105381
16	3.530931	2.399504	1.023282
8	-4.952590	0.394927	-0.313159
8	2.158726	1.739686	1.570499
6	-5.638919	1.639624	-0.162485
1	-4.943674	2.398503	0.216192
1	-6.450081	1.524218	0.565445
6	-6.182115	2.031541	-1.526754
1	-6.870895	1.269030	-1.899481
1	-6.719315	2.983725	-1.461061
1	-5.369122	2.141218	-2.249155
6	1.041382	2.654843	1.863944
1	1.403128	3.404620	2.572617
1	0.757954	3.142560	0.929453
6	-0.083392	1.825510	2.439962
1	0.233042	1.323051	3.356423
1	-0.927007	2.478045	2.678311
1	-0.453346	1.082557	1.733200
6	0.881902	-0.031097	-2.594871
6	0.689356	1.422794	-2.123677
1	-0.096116	-0.459616	-2.833806
1	1.469123	-0.039034	-3.520721
6	0.015260	2.295872	-3.187814
1	0.075911	1.416601	-1.216737
1	1.653611	1.862612	-1.849982
6	-0.219176	3.734521	-2.717019
1	0.634096	2.303700	-4.094554
1	-0.942658	1.844232	-3.472130
1	-0.684566	4.339820	-3.501004
1	-0.880213	3.757135	-1.845319
1	0.722198	4.215383	-2.434007

55

Bu-EtSO4 RCS=2.0

6	1.414726	-0.858126	-1.619915
6	0.900593	-1.682277	-0.718500
6	1.840781	-2.530134	0.140764
6	3.184869	-2.613717	-0.638794
6	1.964508	-1.945214	1.552764
1	0.977325	-1.903943	2.017781
1	2.603296	-2.584126	2.165804
1	2.367682	-0.932026	1.541930
6	4.416929	-2.989850	0.176647
1	5.283009	-3.123969	-0.476859
1	4.234779	-3.937142	0.691370
8	1.400629	-3.893504	0.222733
1	0.470912	-3.888526	0.490474
53	-1.181517	-1.701967	-0.270394
1	3.019888	-3.363895	-1.414043
1	4.667206	-2.231588	0.920873
16	3.407076	-1.019302	-1.552367
1	3.982055	0.371633	0.029325
8	4.381845	0.861153	0.807594
8	-3.786972	-1.488008	0.570558
8	3.412079	2.995263	-0.091990
8	4.371115	2.851532	2.223425
8	-5.551122	-0.400371	1.947869
8	-3.357826	0.728164	1.620058
16	-4.360370	-0.225014	1.101891
16	3.650834	2.239455	1.127599
8	-4.928984	0.475335	-0.329703
8	2.247250	1.624455	1.652682
6	-5.613721	1.720551	-0.172438
1	-4.941319	2.452867	0.290263
1	-6.476940	1.581955	0.488403
6	-6.051846	2.179906	-1.553238
1	-6.717667	1.443152	-2.009963
1	-6.584500	3.134279	-1.483185



S57

1	-5.187069	2.312783	-2.208461
6	1.166091	2.575817	1.954675
1	1.544326	3.288510	2.692482
1	0.919314	3.104061	1.031644
6	-0.002694	1.776740	2.485459
1	0.273589	1.239041	3.394757
1	-0.826602	2.454166	2.723420
1	-0.380185	1.063970	1.751875
6	0.834512	0.107675	-2.595496
6	0.795600	1.568092	-2.108350
1	-0.185524	-0.224745	-2.816300
1	1.399268	0.047856	-3.532801
6	0.214008	2.517724	-3.161369
1	0.187873	1.615052	-1.198585
1	1.800771	1.900487	-1.831725
6	0.129110	3.967366	-2.673992
1	0.830857	2.472355	-4.068218
1	-0.785050	2.170401	-3.451051
1	-0.269068	4.626633	-3.451392
1	-0.527742	4.049070	-1.802528
1	1.114348	4.344259	-2.383469

55

Bu-EtSO4 RCS=2.2

6	1.182229	-0.726803	-1.629083
6	0.665068	-1.583519	-0.778562
6	1.545230	-2.585648	-0.023333
6	2.841263	-2.786910	-0.863119
6	1.788872	-2.098459	1.410357
1	0.831222	-1.968479	1.919253
1	2.367787	-2.841849	1.961577
1	2.311148	-1.141639	1.432378
6	3.999749	-3.451105	-0.122889
1	4.815723	-3.675595	-0.814487
1	3.658432	-4.393103	0.314729
8	0.951998	-3.889993	0.005107
1	0.043495	-3.799454	0.325608
53	-1.420739	-1.485196	-0.278290
1	2.540632	-3.420573	-1.699162
1	4.396242	-2.818690	0.673804
16	3.335294	-1.178782	-1.623815
1	4.139539	-0.048334	-0.009616
8	4.643335	0.354219	0.767564
8	-3.981701	-1.351163	0.492718
8	3.927233	2.634460	-0.000829
8	4.975363	2.267885	2.250070
8	-5.970588	-0.437484	1.668867
8	-3.770242	0.707557	1.878273
16	-4.654321	-0.158021	1.076172
16	4.129687	1.799264	1.172955
8	-4.972787	0.722278	-0.332405
8	2.678681	1.359035	1.756496
6	-5.682790	1.948917	-0.139598
1	-5.110459	2.601932	0.529820
1	-6.651122	1.740156	0.329241
6	-5.864765	2.592050	-1.504284
1	-6.430216	1.932788	-2.167841
1	-6.408646	3.537605	-1.407077
1	-4.895827	2.795532	-1.967446
6	1.759013	2.432981	2.142025
1	2.249133	3.041274	2.907127
1	1.566531	3.046640	1.259461
6	0.500053	1.775660	2.664022
1	0.716403	1.155208	3.535827
1	-0.215785	2.546871	2.960287
1	0.023766	1.156858	1.902249
6	0.751935	0.374062	-2.519035
6	1.031556	1.787289	-1.977481
1	-0.326406	0.249255	-2.676500
1	1.231794	0.249485	-3.496104
6	0.596690	2.882809	-2.956954

S58

1	0.497076	1.909424	-1.029274
1	2.096316	1.897555	-1.751870
6	0.832386	4.295116	-2.413040
1	1.142944	2.759121	-3.900760
1	-0.465642	2.755691	-3.197997
1	0.535059	5.056839	-3.140140
1	0.253021	4.465323	-1.500172
1	1.887153	4.453163	-2.169563

55

Bu-EtSO4 RCS=2.4

6	1.009075	-0.618539	-1.622526
6	0.521197	-1.503839	-0.803609
6	1.369067	-2.574814	-0.101949
6	2.629065	-2.848156	-0.978091
6	1.678192	-2.123114	1.330981
1	0.744032	-1.942195	1.867731
1	2.224136	-2.908806	1.856245
1	2.260465	-1.201778	1.349182
6	3.704047	-3.685023	-0.283159
1	4.480291	-3.971418	-0.996768
1	3.254795	-4.597836	0.117073
8	0.695906	-3.837803	-0.077766
1	-0.186826	-3.704565	0.295175
53	-1.573728	-1.354597	-0.269462
1	2.254518	-3.401587	-1.840983
1	4.182727	-3.141312	0.533767
16	3.315779	-1.280144	-1.659880
1	4.226352	-0.318208	-0.063213
8	4.787682	0.038519	0.708675
8	-4.088510	-1.271551	0.478939
8	4.229920	2.370304	-0.032103
8	5.357072	1.918686	2.163918
8	-6.154872	-0.435006	1.568879
8	-3.988779	0.729575	1.959928
16	-4.811605	-0.108167	1.070972
16	4.425202	1.517340	1.130770
8	-5.055863	0.822844	-0.316680
8	2.969985	1.208033	1.793703
6	-5.784700	2.038555	-0.117542
1	-5.255043	2.667506	0.607392
1	-6.776191	1.806524	0.287393
6	-5.894117	2.731955	-1.464977
1	-6.416761	2.095843	-2.183827
1	-6.449265	3.670290	-1.362645
1	-4.902152	2.957991	-1.864445
6	2.188761	2.359338	2.241653
1	2.772465	2.897420	2.993710
1	2.017903	3.011530	1.382198
6	0.893652	1.822232	2.812155
1	1.085519	1.161129	3.659485
1	0.276066	2.655301	3.158410
1	0.325530	1.271769	2.060673
6	0.703696	0.546218	-2.465708
6	1.153056	1.898719	-1.885514
1	-0.386248	0.546175	-2.604275
1	1.146698	0.396064	-3.456042
6	0.841157	3.067227	-2.826575
1	0.647167	2.053146	-0.926329
1	2.225467	1.871470	-1.672934
6	1.250232	4.423427	-2.244107
1	1.359646	2.908565	-3.780579
1	-0.231128	3.075697	-3.057411
1	1.039646	5.237392	-2.944307
1	0.704571	4.633578	-1.318764
1	2.318581	4.445575	-2.010385

55

Bu-EtSO4 RCS=2.6

6	0.873416	-0.545267	-1.625500
6	0.430364	-1.451769	-0.824475

S59

6	1.257723	-2.547165	-0.129958
6	2.505198	-2.873762	-1.009141
6	1.587041	-2.089676	1.296609
1	0.662068	-1.879394	1.839028
1	2.115804	-2.885305	1.824223
1	2.195181	-1.185379	1.301133
6	3.496884	-3.815937	-0.319700
1	4.252602	-4.150177	-1.034045
1	2.969568	-4.694943	0.060298
8	0.540871	-3.783712	-0.093142
1	-0.321838	-3.626442	0.314963
53	-1.688913	-1.279269	-0.292087
1	2.099331	-3.378585	-1.887835
1	4.013991	-3.328027	0.509094
16	3.341036	-1.363995	-1.648706
1	4.267707	-0.495305	-0.080675
8	4.851656	-0.147156	0.694310
8	-4.162601	-1.238413	0.411370
8	4.365882	2.192592	-0.067843
8	5.548556	1.733106	2.096131
8	-6.275677	-0.446604	1.435014
8	-4.121702	0.650671	2.037516
16	-4.903116	-0.102093	1.044116
16	4.569986	1.346791	1.099671
8	-5.047787	0.924566	-0.284594
8	3.124001	1.116503	1.822207
6	-5.760030	2.143958	-0.042852
1	-5.258938	2.707066	0.752691
1	-6.778183	1.910396	0.287897
6	-5.774708	2.929172	-1.343093
1	-6.268614	2.357405	-2.132722
1	-6.313778	3.872503	-1.207450
1	-4.756311	3.155885	-1.668630
6	2.439493	2.307718	2.312068
1	3.088606	2.803263	3.039459
1	2.268043	2.978488	1.466682
6	1.141003	1.847340	2.940392
1	1.331360	1.166330	3.772233
1	0.594182	2.713763	3.322342
1	0.506281	1.339890	2.212115
6	0.682134	0.640498	-2.458242
6	1.220197	1.948276	-1.850945
1	-0.403018	0.721792	-2.620731
1	1.131661	0.463461	-3.440869
6	1.025774	3.145705	-2.786939
1	0.704069	2.132492	-0.902529
1	2.280927	1.830657	-1.614133
6	1.529995	4.458181	-2.179439
1	1.553626	2.953959	-3.729530
1	-0.036308	3.243957	-3.043722
1	1.404670	5.293003	-2.875465
1	0.980511	4.704028	-1.265136
1	2.590178	4.389162	-1.919831

55

Bu-EtSO4 RCS=2.8

6	0.770460	-0.504427	-1.644032
6	0.384241	-1.422155	-0.846007
6	1.191608	-2.520391	-0.128341
6	2.443417	-2.894943	-0.986116
6	1.514229	-2.035532	1.290310
1	0.588654	-1.802408	1.822680
1	2.029951	-2.826653	1.837038
1	2.135179	-1.140519	1.279166
6	3.352025	-3.907046	-0.276280
1	4.102762	-4.280949	-0.975601
1	2.762186	-4.753377	0.085385
8	0.444613	-3.736961	-0.074884
1	-0.403292	-3.560652	0.355070
53	-1.769672	-1.226380	-0.333999
1	2.031441	-3.370132	-1.878741

S60

1	3.880218	-3.455945	0.566381
16	3.405593	-1.449773	-1.595048
1	4.281667	-0.620607	-0.053021
8	4.861451	-0.253848	0.738230
8	-4.199596	-1.216921	0.329140
8	4.416963	2.071438	-0.086843
8	5.615706	1.654341	2.075502
8	-6.326606	-0.461677	1.342278
8	-4.175973	0.561962	2.077613
16	-4.941429	-0.106443	1.016299
16	4.621249	1.251039	1.099829
8	-5.029449	1.000664	-0.245789
8	3.176751	1.081352	1.851224
6	-5.722478	2.220351	0.053096
1	-5.231709	2.719890	0.895739
1	-6.754239	1.989509	0.340119
6	-5.682233	3.084089	-1.195349
1	-6.165437	2.574186	-2.032432
1	-6.204570	4.029279	-1.015494
1	-4.650234	3.306966	-1.477493
6	2.556295	2.300871	2.348476
1	3.242766	2.774934	3.055728
1	2.389910	2.974447	1.503823
6	1.255937	1.899824	3.013629
1	1.439685	1.216780	3.845379
1	0.755113	2.790647	3.402798
1	0.583220	1.413136	2.305409
6	0.685094	0.673352	-2.493586
6	1.272280	1.955329	-1.875156
1	-0.385722	0.813358	-2.708361
1	1.165602	0.453970	-3.452778
6	1.201057	3.146583	-2.835847
1	0.722040	2.185749	-0.956546
1	2.309986	1.772619	-1.585107
6	1.760870	4.432564	-2.220416
1	1.761290	2.905645	-3.747849
1	0.161454	3.309580	-3.146997
1	1.726384	5.262290	-2.932745
1	1.184398	4.728895	-1.338201
1	2.799590	4.296737	-1.906739

55

Bu-EtSO4 RCS=3.0

6	0.908524	-1.215014	-1.491423
6	0.238889	-1.531212	-0.468225
6	0.574724	-2.114497	0.918143
6	1.829683	-3.047547	0.817217
6	0.729384	-0.944860	1.897592
1	-0.192588	-0.358187	1.926507
1	0.914638	-1.334754	2.899615
1	1.548013	-0.285374	1.612271
6	2.228082	-3.605213	2.191838
1	2.968143	-4.396981	2.060480
1	1.356214	-4.021864	2.702575
8	-0.461890	-2.992372	1.349527
1	-1.289482	-2.497795	1.421571
53	-1.896565	-0.881223	-0.823733
1	1.497656	-3.881124	0.194451
1	2.678474	-2.836175	2.822996
16	3.289133	-2.340414	-0.054004
1	3.955557	-0.989462	0.994835
8	4.453904	-0.269892	1.650221
8	-4.264500	-0.270450	-1.065633
8	4.807963	1.224890	-0.325632
8	5.527715	1.915772	1.971861
8	-6.586411	0.203623	-0.366951
8	-4.943753	-0.664515	1.300063
16	-5.192092	0.093247	0.067489
16	4.609486	1.179730	1.119462
8	-4.666672	1.653164	0.371691
8	3.082572	1.714671	1.425000

## S61

6	-5.357353	2.343748	1.425634
1	-5.252366	1.778217	2.357659
1	-6.421825	2.409850	1.176256
6	-4.735275	3.723238	1.546144
1	-4.837933	4.275857	0.609108
1	-5.231625	4.289888	2.340319
1	-3.672271	3.647475	1.787177
6	2.815896	3.102876	1.101149
1	3.518049	3.732657	1.655109
1	2.974851	3.250500	0.029069
6	1.381000	3.386535	1.498190
1	1.236479	3.224465	2.568395
1	1.136045	4.427730	1.269155
1	0.688699	2.742245	0.952988
6	1.373954	-0.713158	-2.770300
6	2.135613	0.623803	-2.687154
1	0.484028	-0.607051	-3.409114
1	1.995879	-1.483708	-3.238433
6	2.663395	1.073932	-4.052879
1	1.464095	1.386041	-2.277323
1	2.965679	0.518951	-1.984244
6	3.409081	2.409881	-3.980707
1	3.336406	0.303156	-4.448187
1	1.832140	1.152836	-4.765406
1	3.803856	2.698427	-4.959443
1	2.745855	3.211954	-3.640797
1	4.245839	2.351812	-3.279376

55

Bu-EtSO4 RCS=3.2

6	-0.862134	-0.757889	1.344191
6	-0.293397	-1.488514	0.510821
6	-0.505352	-2.473548	-0.631023
6	-1.510453	-3.595265	-0.197812
6	-0.957339	-1.660082	-1.853519
1	-0.217625	-0.885452	-2.074012
1	-1.026676	-2.320544	-2.719289
1	-1.922315	-1.176627	-1.686753
6	-1.866558	-4.521285	-1.367132
1	-2.395986	-5.396976	-0.987576
1	-0.960963	-4.852435	-1.881012
8	0.683367	-3.204764	-0.915840
1	1.376006	-2.596604	-1.204814
53	1.844474	-0.627726	0.895628
1	-0.972378	-4.174235	0.556577
1	-2.522462	-4.023435	-2.083918
16	-3.013989	-3.039526	0.708860
1	-3.518705	-2.161998	-0.207052
8	-4.120642	-0.636016	-1.221733
8	4.112632	-0.061531	1.044040
8	-4.133758	0.906925	0.723484
8	-5.983659	1.000370	-0.930043
8	6.424744	0.228616	0.244161
8	4.734378	-0.880025	-1.228068
16	5.030589	0.083308	-0.164587
16	-4.578320	0.661007	-0.672250
8	4.521255	1.566202	-0.712101
8	-3.669560	1.726771	-1.609186
6	5.177354	2.055618	-1.899426
1	5.026834	1.338435	-2.712404
1	6.250669	2.144922	-1.703007
6	4.562098	3.402687	-2.227981
1	4.709768	4.105776	-1.405070
1	5.030069	3.815923	-3.126685
1	3.489717	3.303602	-2.410257
6	-3.981106	3.116854	-1.450193
1	-5.034661	3.282121	-1.697893
1	-3.824379	3.410666	-0.405395
6	-3.067571	3.898176	-2.378827
1	-3.226543	3.596513	-3.417039
1	-3.272196	4.970284	-2.293337

S62

1	-2.017984	3.724998	-2.128501
6	-1.541984	0.141274	2.240436
6	-1.113581	1.622068	2.135841
1	-1.478370	-0.226216	3.270416
1	-2.597136	0.086057	1.914263
6	-2.008951	2.517453	2.997077
1	-0.065564	1.724706	2.435661
1	-1.184916	1.928861	1.088936
6	-1.605382	3.992875	2.924706
1	-3.044027	2.396011	2.664267
1	-1.966824	2.179240	4.040509
1	-2.259267	4.612093	3.545826
1	-0.576509	4.144586	3.267589
1	-1.671082	4.367658	1.898629

55

Bu-EtSO4 RCS=3.4

6	-0.696804	-0.684110	1.320571
6	-0.304067	-1.506215	0.479513
6	-0.570247	-2.492559	-0.642261
6	-1.524213	-3.637816	-0.155949
6	-1.111499	-1.685465	-1.832776
1	-0.395741	-0.903561	-2.102009
1	-1.231435	-2.348153	-2.691186
1	-2.068164	-1.211416	-1.602629
6	-1.906484	-4.579381	-1.304758
1	-2.394647	-5.465674	-0.895510
1	-1.018218	-4.890385	-1.859743
8	0.614639	-3.200372	-1.004033
1	1.269582	-2.577526	-1.343487
53	1.923226	-0.690647	0.830616
1	-0.935381	-4.197912	0.574410
1	-2.609628	-4.103836	-1.991266
16	-3.006038	-3.128314	0.817280
1	-3.546748	-2.228203	-0.052256
8	-4.194823	-0.658659	-1.026560
8	4.191299	-0.244624	0.920606
8	-3.901431	1.016515	0.783580
8	-6.056692	0.899055	-0.443955
8	6.461279	0.137092	0.049745
8	4.683236	-0.741480	-1.474965
16	5.048718	0.063112	-0.307808
16	-4.608978	0.648779	-0.468522
8	4.531016	1.608925	-0.610964
8	-3.984261	1.690775	-1.637122
6	5.113094	2.252886	-1.764115
1	4.892887	1.656255	-2.654609
1	6.198759	2.304265	-1.633277
6	4.501764	3.637698	-1.858626
1	4.719701	4.218551	-0.959566
1	4.913839	4.167072	-2.723042
1	3.417714	3.574396	-1.975901
6	-4.312143	3.075598	-1.471753
1	-5.400801	3.193910	-1.480794
1	-3.936592	3.428047	-0.503744
6	-3.666561	3.837380	-2.616602
1	-4.041736	3.476943	-3.577650
1	-3.893198	4.905315	-2.533494
1	-2.581025	3.711407	-2.603249
6	-1.284565	0.257705	2.246337
6	-0.914134	1.734864	2.006420
1	-1.075347	-0.048311	3.277315
1	-2.367617	0.151569	2.063622
6	-1.710768	2.664001	2.926731
1	0.161205	1.875341	2.159159
1	-1.134808	1.978227	0.963973
6	-1.357109	4.139388	2.719532
1	-2.776967	2.507833	2.737799
1	-1.526003	2.388561	3.973301
1	-1.939896	4.783306	3.384839
1	-0.296420	4.328671	2.915617

S63

1 -1.565213 4.450687 1.691289

55

Bu-EtSO4 RCS=3.6

6	-0.566497	-0.710633	1.438953
6	-0.368006	-1.549292	0.559373
6	-0.613334	-2.493189	-0.592098
6	-1.599588	-3.638384	-0.173164
6	-1.096578	-1.650978	-1.783145
1	-0.357979	-0.877078	-2.010141
1	-1.197784	-2.293805	-2.658771
1	-2.052509	-1.165094	-1.576498
6	-1.940272	-4.551670	-1.357330
1	-2.453329	-5.440643	-0.985657
1	-1.033390	-4.860997	-1.882202
8	0.576909	-3.212386	-0.926374
1	1.245330	-2.592250	-1.243856
53	1.956394	-0.675833	0.857980
1	-1.045047	-4.218544	0.568116
1	-2.611375	-4.055698	-2.061123
16	-3.125386	-3.145902	0.745014
1	-3.608773	-2.187610	-0.099279
8	-4.219380	-0.622004	-1.074819
8	4.200480	-0.246106	0.848830
8	-3.795656	1.064513	0.697987
8	-6.033364	0.939211	-0.368351
8	6.424581	0.124031	-0.131297
8	4.574350	-0.762933	-1.565005
16	4.998783	0.052879	-0.427203
16	-4.590269	0.689191	-0.493591
8	4.467174	1.593412	-0.712720
8	-4.054271	1.722497	-1.715308
6	4.978161	2.227442	-1.906340
1	4.706165	1.620705	-2.775131
1	6.069417	2.282006	-1.840159
6	4.357950	3.609374	-1.976918
1	4.627942	4.199751	-1.098496
1	4.715873	4.130736	-2.869749
1	3.269134	3.542066	-2.028480
6	-4.364215	3.108448	-1.532937
1	-5.450368	3.231811	-1.464455
1	-3.918990	3.463769	-0.595946
6	-3.799302	3.863823	-2.723967
1	-4.242824	3.500831	-3.654518
1	-4.015914	4.932968	-2.629593
1	-2.715963	3.733788	-2.786923
6	-1.058389	0.205441	2.457501
6	-0.766112	1.693995	2.195398
1	-0.686928	-0.105041	3.440628
1	-2.146689	0.054810	2.437760
6	-1.448860	2.589064	3.233503
1	0.315900	1.863959	2.202550
1	-1.139359	1.943776	1.199945
6	-1.164415	4.076231	3.005053
1	-2.527997	2.411753	3.191950
1	-1.116266	2.304398	4.240531
1	-1.664623	4.695734	3.755415
1	-0.091586	4.290107	3.056014
1	-1.520847	4.394331	2.020820

55

Bu-EtSO4 RCS=3.8

6	-0.472641	0.298908	0.086419
6	-0.403773	-0.862708	-0.335657
6	-0.942564	-2.096491	-1.007368
6	-1.059123	-3.292765	-0.013630
6	-2.270552	-1.705817	-1.675986
1	-2.104474	-0.871012	-2.362641
1	-2.641596	-2.556352	-2.249784
1	-3.027427	-1.399704	-0.951575
6	-1.683646	-4.529766	-0.668212

S64

1	-1.568714	-5.385667	-0.000849
1	-1.189385	-4.755522	-1.616659
8	-0.008624	-2.558159	-1.993670
1	0.073709	-1.885005	-2.678609
53	1.948112	-0.672118	0.252565
1	-0.031338	-3.529676	0.271611
1	-2.752083	-4.391611	-0.845093
16	-1.853400	-2.897714	1.607966
1	-2.975546	-2.279545	1.157731
8	-4.524188	-0.978900	0.616616
8	4.179225	-0.956219	0.740069
8	-3.802260	1.355874	0.179857
8	-5.468392	0.902372	1.963961
8	6.621681	-0.860297	0.479172
8	5.160820	-0.567681	-1.528520
16	5.350076	-0.420968	-0.086130
16	-4.867482	0.455942	0.698844
8	5.190687	1.197775	0.254513
8	-6.092804	0.552288	-0.450781
6	6.161378	2.064318	-0.367490
1	6.089517	1.959738	-1.454636
1	7.164455	1.761780	-0.050202
6	5.847313	3.480706	0.075343
1	5.910087	3.568484	1.162325
1	6.563015	4.177271	-0.371779
1	4.841575	3.769838	-0.237961
6	-6.704509	1.839772	-0.594959
1	-7.134540	2.146772	0.364535
1	-5.943205	2.574046	-0.882742
6	-7.777425	1.717714	-1.663582
1	-8.527697	0.978150	-1.372853
1	-8.276692	2.681442	-1.807980
1	-7.340651	1.407189	-2.616191
6	-0.763203	1.621031	0.599126
6	-0.161850	2.785418	-0.207678
1	-0.461776	1.671980	1.651443
1	-1.868902	1.663948	0.578771
6	-0.586376	4.143170	0.361071
1	0.930654	2.706147	-0.212939
1	-0.492784	2.703292	-1.248439
6	-0.022253	5.322887	-0.435441
1	-1.680124	4.196762	0.379920
1	-0.256735	4.215804	1.404613
1	-0.338343	6.278319	-0.006772
1	1.072397	5.308174	-0.446553
1	-0.364305	5.296402	-1.475022

55

Bu-EtSO4 RCS=4.0

6	-0.475486	0.365741	-0.070731
6	-0.481661	-0.823590	-0.413359
6	-1.026605	-2.057475	-1.078705
6	-1.050152	-3.302311	-0.139569
6	-2.400682	-1.686394	-1.659570
1	-2.297072	-0.828672	-2.329838
1	-2.780556	-2.531748	-2.235250
1	-3.121285	-1.417293	-0.885645
6	-1.627120	-4.538902	-0.838702
1	-1.451910	-5.416957	-0.214504
1	-1.146563	-4.695643	-1.807574
8	-0.132480	-2.445509	-2.135287
1	-0.117162	-1.742494	-2.794560
53	1.894559	-0.675037	0.194903
1	-0.003780	-3.498067	0.105711
1	-2.705568	-4.449527	-0.983145
16	-1.822760	-3.046060	1.524407
1	-2.931020	-2.357326	1.151631
8	-4.467965	-0.943374	0.777835
8	4.099309	-1.035424	0.718956
8	-3.765087	1.344970	0.119210
8	-5.214332	1.034695	2.110893



S65

8	6.548631	-0.983097	0.524982
8	5.148325	-0.458753	-1.479022
16	5.304471	-0.455783	-0.025525
16	-4.775020	0.501108	0.813296
8	5.176992	1.125859	0.466413
8	-6.127687	0.559508	-0.187539
6	6.195381	2.017833	-0.031420
1	6.163453	2.022185	-1.125524
1	7.176160	1.653984	0.290860
6	5.903821	3.393378	0.537504
1	5.926089	3.372264	1.629370
1	6.655938	4.107123	0.187903
1	4.919702	3.743703	0.218086
6	-6.735861	1.848453	-0.329648
1	-7.049469	2.212625	0.654679
1	-6.003845	2.553192	-0.741049
6	-7.925512	1.691220	-1.261432
1	-8.646271	0.980992	-0.848524
1	-8.426603	2.655041	-1.398946
1	-7.604388	1.324473	-2.239724
6	-0.709067	1.729927	0.363432
6	-0.084636	2.814445	-0.531648
1	-0.373892	1.836281	1.401176
1	-1.811298	1.808332	0.374107
6	-0.428208	4.223003	-0.036493
1	1.002528	2.685149	-0.565523
1	-0.452439	2.685160	-1.555275
6	0.159032	5.324065	-0.923786
1	-1.517204	4.329580	0.014813
1	-0.059279	4.344170	0.989160
1	-0.097578	6.317830	-0.545505
1	1.250699	5.256614	-0.970704
1	-0.221207	5.250387	-1.947713

55

Bu-EtSO4 RCS=4.2

6	-0.478543	0.397451	-0.164756
6	-0.541845	-0.807064	-0.444414
6	-1.093896	-2.042827	-1.102705
6	-1.048645	-3.325490	-0.213543
6	-2.497987	-1.688857	-1.618172
1	-2.437810	-0.823436	-2.283631
1	-2.889441	-2.535353	-2.184368
1	-3.186551	-1.434545	-0.811192
6	-1.537405	-4.564259	-0.975659
1	-1.331554	-5.453974	-0.377618
1	-1.023650	-4.659412	-1.934767
8	-0.232441	-2.372743	-2.208339
1	-0.248817	-1.638421	-2.832552
53	1.860969	-0.683682	0.152687
1	0.004556	-3.467846	0.037691
1	-2.615112	-4.528818	-1.146511
16	-1.869949	-3.220848	1.451379
1	-2.920176	-2.422274	1.138305
8	-4.400396	-0.879787	0.914583
8	4.050524	-1.090950	0.678823
8	-3.725229	1.363761	0.091952
8	-5.035613	1.172649	2.191523
8	6.501555	-1.039082	0.515704
8	5.126820	-0.326785	-1.448032
16	5.267803	-0.454725	0.001209
16	-4.691480	0.567823	0.896319
8	5.143749	1.076255	0.631980
8	-6.110397	0.591996	-0.010787
6	6.172174	2.003580	0.227279
1	6.148567	2.110705	-0.861779
1	7.147869	1.603756	0.520959
6	5.885165	3.321524	0.921068
1	5.899915	3.197797	2.006199
1	6.643991	4.059807	0.644609
1	4.905346	3.706860	0.630044

S66

6	-6.718590	1.878260	-0.172827
1	-6.961230	2.292185	0.811904
1	-6.012425	2.555682	-0.667138
6	-7.970751	1.688374	-1.012093
1	-8.665690	1.005549	-0.516883
1	-8.474122	2.649300	-1.161196
1	-7.720300	1.272295	-1.991302
6	-0.664696	1.789202	0.206478
6	-0.031941	2.806509	-0.758801
1	-0.296023	1.937353	1.227480
1	-1.762596	1.898971	0.244205
6	-0.310460	4.248905	-0.323794
1	1.048530	2.637089	-0.819173
1	-0.435938	2.641890	-1.763641
6	0.284603	5.283888	-1.282560
1	-1.392880	4.397438	-0.243759
1	0.095888	4.406219	0.682605
1	0.075550	6.303430	-0.945885
1	1.371023	5.174439	-1.360781
1	-0.131961	5.174787	-2.289040

55

Bu-EtSO4 RCS=4.4

6	-0.723859	0.706871	-0.352596
6	-0.607134	-0.430205	-0.822913
6	-1.001988	-1.742935	-1.441394
6	-0.537413	-2.956048	-0.562119
6	-2.511968	-1.699136	-1.720560
1	-2.714343	-0.936656	-2.478922
1	-2.830910	-2.670059	-2.104241
1	-3.089027	-1.453392	-0.831024
6	-0.341241	-4.234644	-1.385860
1	-0.040732	-5.047862	-0.720045
1	0.434444	-4.094166	-2.137613
8	-0.284522	-1.888786	-2.680703
1	-0.480087	-1.121471	-3.229990
53	1.813658	0.175865	-0.789289
1	0.422386	-2.682217	-0.123148
1	-1.264604	-4.534126	-1.886927
16	-1.675024	-3.423571	0.832525
1	-2.081268	-2.187555	1.222683
8	-2.988211	-0.365491	1.411969
8	4.076916	0.291470	-1.046220
8	-4.082174	1.837635	1.181026
8	-5.018401	0.169971	2.772483
8	6.432938	0.651572	-0.458283
8	4.647486	1.771879	0.887711
16	5.072950	0.638074	0.068932
16	-4.242122	0.409307	1.549718
8	4.905923	-0.720658	0.998521
8	-5.153181	-0.260797	0.293951
6	5.632307	-0.727750	2.246984
1	5.299661	0.117695	2.856106
1	6.701097	-0.614490	2.037895
6	5.339315	-2.052223	2.924937
1	5.667624	-2.886988	2.301656
1	5.867739	-2.103422	3.881693
1	4.269234	-2.160554	3.114212
6	-6.499572	0.216981	0.182408
1	-7.037402	0.002852	1.112066
1	-6.489104	1.302888	0.032713
6	-7.141985	-0.490942	-0.998220
1	-7.138195	-1.573255	-0.846720
1	-8.179145	-0.160524	-1.115945
1	-6.602256	-0.271211	-1.923008
6	-1.013527	2.000425	0.236071
6	-0.797580	3.201405	-0.702986
1	-0.424261	2.110269	1.153048
1	-2.069228	1.947209	0.551475
6	-1.178024	4.520574	-0.022681
1	0.247730	3.236638	-1.028079

S67

1	-1.408135	3.063155	-1.602306
6	-1.003463	5.732886	-0.941501
1	-2.215584	4.459230	0.321905
1	-0.562198	4.651544	0.875088
1	-1.277080	6.660396	-0.430159
1	0.033842	5.831196	-1.277609
1	-1.634329	5.647184	-1.832343

55

Bu-EtSO4 RCS=4.6

6	-0.659128	0.669586	-0.396481
6	-0.638161	-0.495113	-0.810200
6	-1.111803	-1.810655	-1.366705
6	-0.759636	-3.005797	-0.393286
6	-2.605545	-1.669132	-1.695249
1	-2.727259	-0.928532	-2.492196
1	-2.983462	-2.631971	-2.043621
1	-3.186640	-1.342270	-0.835086
6	-0.353098	-4.278675	-1.147011
1	-0.134648	-5.067080	-0.422451
1	0.534382	-4.103914	-1.753475
8	-0.381564	-2.069953	-2.579500
1	-0.545626	-1.338423	-3.185040
53	1.824318	-0.034567	-0.800772
1	0.084164	-2.687564	0.218541
1	-1.154114	-4.628986	-1.801896
16	-2.104790	-3.536950	0.780522
1	-2.470716	-2.312410	1.244289
8	-3.014285	-0.345762	1.410326
8	4.093595	-0.089167	-1.045967
8	-3.901321	1.952825	1.200666
8	-4.972510	0.369928	2.792971
8	6.458152	0.356371	-0.556705
8	4.698032	1.818945	0.452561
16	5.098100	0.505832	-0.051015
16	-4.188184	0.543315	1.563958
8	4.902839	-0.569092	1.192222
8	-5.169333	-0.032470	0.313528
6	5.647118	-0.284994	2.396847
1	5.346211	0.695463	2.777475
1	6.715249	-0.259054	2.157777
6	5.329259	-1.388416	3.387383
1	5.625731	-2.361826	2.990354
1	5.870459	-1.214301	4.322278
1	4.259598	-1.414515	3.606128
6	-6.467409	0.566831	0.218486
1	-7.013790	0.395912	1.152107
1	-6.359370	1.648359	0.075780
6	-7.182700	-0.070940	-0.960212
1	-7.276177	-1.150166	-0.815667
1	-8.186453	0.353460	-1.065576
1	-6.633671	0.105277	-1.888822
6	-0.873835	1.997662	0.148848
6	-0.632673	3.149338	-0.843883
1	-0.250416	2.117277	1.041634
1	-1.920767	2.001337	0.498300
6	-0.926428	4.511657	-0.207202
1	0.402103	3.120433	-1.201837
1	-1.278100	3.005992	-1.717678
6	-0.724126	5.676328	-1.180378
1	-1.953897	4.515901	0.171643
1	-0.275575	4.647618	0.664721
1	-0.935739	6.635953	-0.699789
1	0.305123	5.709496	-1.551965
1	-1.387297	5.586356	-2.047007

55

Bu-EtSO4 RCS=4.8

6	-0.721383	0.219193	0.745515
6	-0.097134	-0.690105	0.170706
6	-0.236131	-2.090708	-0.407638

S68

6	-1.093899	-2.863824	0.642553
6	-0.899085	-1.934995	-1.782918
1	-0.295537	-1.271999	-2.410700
1	-0.963495	-2.915709	-2.254571
1	-1.899735	-1.512413	-1.677396
6	-0.285149	-3.248483	1.882966
1	-0.955678	-3.635766	2.651821
1	0.241614	-2.378956	2.285637
8	1.010310	-2.756999	-0.509911
1	1.556339	-2.303124	-1.162558
53	1.837321	0.589739	-0.157325
1	-1.922758	-2.212140	0.908816
1	0.461960	-4.009142	1.650826
16	-1.915835	-4.363428	-0.044130
1	-3.053287	-3.727700	-0.396135
8	-3.647620	-1.218136	-0.027653
8	3.853108	1.551759	-0.792615
8	-4.483509	0.615899	1.406687
8	-6.062229	-1.131440	0.610128
8	6.250418	2.098723	-0.764766
8	5.113587	1.448807	1.364179
16	5.195700	1.345730	-0.092608
16	-4.812767	-0.398737	0.370724
8	5.429516	-0.260749	-0.445982
8	-5.066463	0.491424	-1.036523
6	6.607804	-0.864532	0.126785
1	6.557266	-0.780978	1.216579
1	7.492820	-0.325825	-0.227427
6	6.629767	-2.314390	-0.318510
1	6.671301	-2.383888	-1.407928
1	7.509482	-2.816663	0.095249
1	5.736732	-2.838666	0.028938
6	-6.238792	1.317595	-1.046370
1	-7.123992	0.690894	-0.897341
1	-6.184614	2.037917	-0.221646
6	-6.286327	2.026815	-2.388671
1	-6.331700	1.301988	-3.205217
1	-7.171882	2.668099	-2.443768
1	-5.399315	2.649139	-2.531475
6	-1.462190	1.266270	1.391097
6	-1.675093	2.538607	0.543104
1	-1.012234	1.498775	2.363538
1	-2.463635	0.827898	1.589820
6	-2.540025	3.562547	1.284168
1	-0.703937	2.974729	0.285416
1	-2.163190	2.250882	-0.392492
6	-2.787149	4.828579	0.459105
1	-3.492561	3.090872	1.543420
1	-2.052057	3.833497	2.229197
1	-3.404539	5.544846	1.009224
1	-1.847483	5.327832	0.200300
1	-3.305692	4.592671	-0.475351

55

Bu-EtSO4 RCS=5.0

6	-0.725584	0.244638	0.692840
6	-0.130155	-0.712764	0.174274
6	-0.158724	-2.117472	-0.405576
6	-1.065950	-2.962366	0.540532
6	-0.708790	-1.993139	-1.833801
1	-0.083635	-1.309690	-2.415761
1	-0.692283	-2.977021	-2.302967
1	-1.729667	-1.606833	-1.811178
6	-0.430885	-3.190485	1.913870
1	-1.154388	-3.664078	2.579084
1	-0.122647	-2.240736	2.358773
8	1.125806	-2.721077	-0.392116
1	1.725267	-2.198567	-0.938436
53	1.806609	0.647390	-0.148343
1	-2.009103	-2.426036	0.632784
1	0.452453	-3.827539	1.842177

S69

16	-1.505937	-4.616739	-0.184185
1	-2.695263	-4.240026	-0.694943
8	-3.452987	-1.000369	-0.102785
8	3.803100	1.629216	-0.762228
8	-4.489735	0.572612	1.500974
8	-5.811536	-1.350430	0.639833
8	6.202083	2.163080	-0.736903
8	5.064977	1.521515	1.394959
16	5.146649	1.415611	-0.060998
16	-4.709472	-0.407558	0.406674
8	5.368418	-0.191866	-0.413345
8	-5.178605	0.522749	-0.917210
6	6.540733	-0.805705	0.162840
1	6.488317	-0.720092	1.252278
1	7.430748	-0.274883	-0.190556
6	6.550871	-2.256057	-0.280807
1	6.592938	-2.327364	-1.370053
1	7.426165	-2.764749	0.134366
1	5.653691	-2.773054	0.066814
6	-6.456532	1.163133	-0.802419
1	-7.228608	0.403680	-0.641299
1	-6.450508	1.836718	0.062516
6	-6.700751	1.929931	-2.090677
1	-6.697631	1.252371	-2.948091
1	-7.671678	2.434153	-2.049767
1	-5.925689	2.684514	-2.246880
6	-1.452153	1.330679	1.301309
6	-1.751258	2.518085	0.363846
1	-0.932237	1.656768	2.209998
1	-2.418667	0.892202	1.614794
6	-2.587128	3.588963	1.071385
1	-0.811070	2.947864	0.001245
1	-2.296304	2.139630	-0.505457
6	-2.919992	4.772322	0.158428
1	-3.509315	3.125875	1.435440
1	-2.043461	3.951049	1.953545
1	-3.517358	5.522934	0.684542
1	-2.011967	5.264328	-0.205944
1	-3.492591	4.443884	-0.714383

55

Bu-EtSO4 RCS=5.2

6	-0.670511	0.335298	0.676739
6	-0.191307	-0.706569	0.208172
6	-0.159313	-2.107967	-0.383182
6	-1.110612	-3.020741	0.458400
6	-0.607076	-1.976879	-1.846799
1	0.050186	-1.285463	-2.381127
1	-0.550422	-2.957525	-2.319553
1	-1.630283	-1.598064	-1.890692
6	-0.642112	-3.183291	1.904815
1	-1.389850	-3.736646	2.474382
1	-0.507268	-2.205641	2.375204
8	1.137060	-2.682963	-0.278708
1	1.769165	-2.123652	-0.746572
53	1.803487	0.698265	-0.140597
1	-2.099374	-2.564832	0.424124
1	0.308514	-3.717288	1.957307
16	-1.302760	-4.735351	-0.292967
1	-2.507132	-4.509798	-0.854479
8	-3.410300	-0.913432	-0.135227
8	3.800611	1.627493	-0.767996
8	-4.425701	0.668790	1.477354
8	-5.663518	-1.387998	0.827683
8	6.211170	2.099052	-0.758426
8	5.063933	1.534803	1.390635
16	5.141829	1.393059	-0.061720
16	-4.658636	-0.381961	0.454146
8	5.317325	-0.225627	-0.379280
8	-5.308242	0.439414	-0.865804
6	6.472581	-0.861271	0.210144

S70

1	6.421460	-0.752933	1.297497
1	7.376694	-0.361913	-0.152881
6	6.442318	-2.319275	-0.205967
1	6.482393	-2.412535	-1.293573
1	7.303416	-2.843574	0.219217
1	5.531680	-2.805120	0.151306
6	-6.606445	1.011084	-0.660360
1	-7.312655	0.219021	-0.389799
1	-6.562155	1.729627	0.166418
6	-7.015552	1.692631	-1.954843
1	-7.050319	0.971334	-2.775148
1	-8.007571	2.142963	-1.845864
1	-6.305394	2.479951	-2.220097
6	-1.378391	1.463282	1.246966
6	-1.678606	2.601976	0.253120
1	-0.836297	1.833343	2.124599
1	-2.340784	1.048857	1.595153
6	-2.523725	3.701034	0.904616
1	-0.740257	3.019989	-0.127906
1	-2.219061	2.179623	-0.598799
6	-2.858471	4.838053	-0.064791
1	-3.445653	3.250368	1.284779
1	-1.987259	4.107217	1.771895
1	-3.462999	5.609161	0.422138
1	-1.951291	5.317788	-0.447351
1	-3.424586	4.465297	-0.923923

55

Bu-EtSO4 RCS=5.4

6	-0.599931	0.421608	0.739777
6	-0.288355	-0.701005	0.314563
6	-0.169692	-2.097864	-0.289575
6	-1.141572	-3.097239	0.440281
6	-0.504516	-1.964048	-1.782770
1	0.173377	-1.253604	-2.262628
1	-0.388092	-2.939543	-2.255530
1	-1.530716	-1.609498	-1.899885
6	-0.824961	-3.235015	1.928104
1	-1.576361	-3.860746	2.411045
1	-0.838631	-2.252859	2.409079
8	1.140151	-2.618429	-0.082494
1	1.784225	-2.021331	-0.483313
53	1.782914	0.791206	-0.082977
1	-2.152239	-2.716739	0.299880
1	0.160265	-3.677529	2.087217
16	-1.132740	-4.846071	-0.327775
1	-2.298428	-4.705734	-0.989676
8	-3.394706	-0.979547	-0.191188
8	3.773328	1.671669	-0.744426
8	-4.346541	0.683244	1.384368
8	-5.622649	-1.383526	0.855881
8	6.201581	2.022423	-0.818447
8	5.109194	1.482504	1.365791
16	5.128091	1.358112	-0.089347
16	-4.616378	-0.405965	0.412826
8	5.206062	-0.260851	-0.435591
8	-5.295985	0.369273	-0.922119
6	6.345833	-0.967621	0.103453
1	6.338578	-0.873183	1.193154
1	7.261866	-0.511660	-0.285569
6	6.221297	-2.414906	-0.331464
1	6.217238	-2.493237	-1.420917
1	7.067600	-2.990924	0.054553
1	5.299636	-2.857593	0.052567
6	-6.574538	0.975550	-0.698894
1	-7.286967	0.210792	-0.371371
1	-6.488961	1.727571	0.094255
6	-7.014150	1.610174	-2.007361
1	-7.090808	0.855680	-2.794339
1	-7.992873	2.085725	-1.885400
1	-6.297730	2.370146	-2.329576

S71

6	-1.309352	1.569846	1.296391
6	-1.634094	2.668911	0.267850
1	-0.745876	1.977339	2.142563
1	-2.259611	1.160925	1.672525
6	-2.492126	3.775802	0.888602
1	-0.706680	3.090008	-0.136137
1	-2.176018	2.210677	-0.564425
6	-2.848034	4.877200	-0.113901
1	-3.406467	3.323607	1.285050
1	-1.958947	4.216506	1.741014
1	-3.463063	5.653512	0.351230
1	-1.949702	5.358955	-0.514451
1	-3.410962	4.469157	-0.958924

53

Ph-EtSO4 lec

6	-2.077300	4.493401	-2.613898
6	-2.441992	3.150166	-2.698196
6	-1.917558	2.221790	-1.806142
6	-1.032405	2.661661	-0.799214
6	-0.679070	4.024460	-0.706310
6	-1.194555	4.929700	-1.620038
1	-2.486244	5.208889	-3.319252
1	-3.143023	2.818851	-3.455075
1	-2.214996	1.176361	-1.830471
1	0.001959	4.347151	0.071850
1	-0.918065	5.975996	-1.558862
6	-0.550103	1.721168	0.134591
6	-0.167286	0.854509	0.938717
6	-0.547174	-0.170344	2.004484
6	-1.898961	0.319667	2.615750
6	-0.645531	-1.526319	1.295885
1	0.321671	-1.786439	0.856091
1	-0.921719	-2.282674	2.030162
1	-1.394378	-1.492554	0.501370
6	-1.738135	1.595313	3.446910
1	-2.721895	1.965494	3.738984
1	-1.228238	2.377354	2.877135
8	0.403979	-0.191297	3.055463
1	1.205588	-0.630765	2.746625
53	2.087254	0.888309	0.181878
1	-2.590091	0.479716	1.788420
1	-1.154073	1.404342	4.348745
16	-2.734753	-0.978348	3.644267
1	-3.638942	-1.293819	2.687734
8	-4.495369	-0.574816	0.780028
8	4.350972	0.711303	-0.223970
8	-2.943150	-0.664264	-1.154224
8	-5.355842	-0.254560	-1.544419
8	6.585886	-0.310813	-0.183407
8	4.748317	-1.307069	1.191962
16	5.161372	-0.568725	-0.001858
16	-4.337009	-0.845434	-0.660787
8	4.640893	-1.440474	-1.310043
8	-4.592159	-2.505807	-0.711127
6	5.163731	-2.781679	-1.423469
1	4.885760	-3.348778	-0.530036
1	6.255654	-2.734092	-1.486298
6	4.563729	-3.389365	-2.676739
1	4.840735	-2.807978	-3.559002
1	4.930236	-4.412356	-2.804809
1	3.474084	-3.417719	-2.608654
6	-4.546429	-3.104011	-2.012759
1	-5.319952	-2.655110	-2.645317
1	-3.569484	-2.907450	-2.468811
6	-4.776980	-4.595079	-1.836867
1	-5.748606	-4.782465	-1.372881
1	-4.753330	-5.097005	-2.809661
1	-4.002966	-5.033073	-1.201808

Ph-EtSO4 1r

6	2.098165	-2.988839	-3.763857
6	2.918855	-1.961186	-3.302805
6	2.778523	-1.477757	-2.004053
6	1.805478	-2.010730	-1.145214
6	0.991198	-3.051059	-1.616335
6	1.135757	-3.532389	-2.914126
1	2.207291	-3.363485	-4.775875
1	3.670397	-1.527566	-3.953456
1	3.419555	-0.669494	-1.672019
1	0.244667	-3.481657	-0.961994
1	0.492693	-4.334016	-3.260305
6	1.663171	-1.514332	0.239065
6	0.575828	-1.180182	0.948524
6	0.821740	-0.676880	2.376666
6	2.217628	-1.225591	2.774805
6	0.707020	0.852453	2.434043
1	-0.294433	1.153474	2.119930
1	0.860295	1.199689	3.457841
1	1.426870	1.340442	1.774178
6	2.961808	-0.495633	3.885131
1	3.890656	-1.016103	4.133629
1	2.337971	-0.476980	4.782709
8	-0.070292	-1.265328	3.328331
1	-0.977670	-1.122519	3.021807
53	-1.424847	-1.102256	0.239146
1	2.048946	-2.263559	3.068315
1	3.209515	0.531983	3.613227
16	3.194259	-1.331071	1.205366
1	3.875921	0.721251	0.951982
8	4.228407	1.660002	0.971772
8	-3.987374	-0.920783	-0.623681
8	4.443956	1.563601	-1.527461
8	4.578927	3.734060	-0.272667
8	-6.406481	-0.348023	-0.603114
8	-5.010302	0.081447	1.412274
16	-5.069458	-0.077024	-0.052472
16	4.024055	2.407075	-0.418549
8	-4.629099	1.437285	-0.674740
8	2.403463	2.465477	-0.394630
6	-5.506897	2.513008	-0.334265
1	-5.563940	2.608496	0.756483
1	-6.512836	2.297719	-0.712766
6	-4.948044	3.778803	-0.962984
1	-4.888495	3.675129	-2.049575
1	-5.592275	4.633333	-0.730171
1	-3.944800	3.987829	-0.582436
6	1.726165	2.856995	-1.636224
1	2.101864	3.839842	-1.933722
1	1.978302	2.122775	-2.403542
6	0.243233	2.885119	-1.339579
1	0.013718	3.613185	-0.559238
1	-0.298800	3.168550	-2.245839
1	-0.117635	1.904848	-1.024830

53

Ph-SO4 RCS=1.8

6	1.800125	3.785615	-2.288836
6	0.998065	3.463793	-1.194763
6	0.789187	2.133727	-0.841102
6	1.373229	1.096004	-1.582587
6	2.192083	1.433055	-2.672174
6	2.398443	2.763706	-3.024839
1	1.956294	4.822575	-2.565818
1	0.528063	4.249349	-0.613422
1	0.168379	1.896041	0.012220
1	2.657331	0.644322	-3.251645
1	3.023636	3.001088	-3.878859
6	1.148964	-0.319608	-1.222831
6	0.027447	-0.969670	-0.871575
6	0.212078	-2.436112	-0.453303



S73

6	1.510430	-2.902724	-1.160568
6	0.261032	-2.530915	1.079699
1	-0.664449	-2.129670	1.497679
1	0.350604	-3.574814	1.387410
1	1.096996	-1.961690	1.494279
6	2.231388	-4.106935	-0.570534
1	3.086490	-4.388147	-1.190994
1	1.543599	-4.956141	-0.541522
8	-0.799311	-3.305278	-0.960266
1	-1.664246	-2.898282	-0.799785
53	-1.943533	-0.187806	-0.792779
1	1.221023	-3.115684	-2.191606
1	2.594115	-3.918905	0.441668
16	2.587131	-1.401334	-1.262150
1	3.556165	-1.276658	0.655351
8	3.989771	-1.313162	1.560143
8	-4.470759	0.763953	-0.720717
8	6.100934	-0.472959	0.487886
8	5.812030	-0.518968	2.982112
8	-6.917768	0.840086	-0.289670
8	-5.623201	-1.215194	0.254116
16	-5.619790	0.247538	0.068770
16	5.249871	-0.352687	1.659919
8	-5.244260	0.883084	1.593348
8	4.447543	1.061067	1.571707
6	-6.185245	0.584936	2.627421
1	-6.274164	-0.502032	2.739590
1	-7.168857	0.983374	2.352719
6	-5.676628	1.224991	3.908610
1	-5.585936	2.307678	3.788249
1	-6.368828	1.023391	4.733104
1	-4.694376	0.826202	4.174992
6	5.257930	2.264636	1.421431
1	5.963643	2.315923	2.255563
1	5.812208	2.190711	0.483107
6	4.300417	3.437087	1.424137
1	3.750907	3.487233	2.366211
1	4.865140	4.365793	1.301390
1	3.584619	3.355216	0.604379

53

Ph-SO4 RCS=2.0

6	1.968019	3.761966	-2.493500
6	1.053294	3.508251	-1.472378
6	0.786902	2.202277	-1.071811
6	1.426376	1.117996	-1.695582
6	2.356882	1.387868	-2.712843
6	2.620826	2.694834	-3.109650
1	2.170791	4.780776	-2.805278
1	0.540414	4.329038	-0.983175
1	0.077545	2.019146	-0.276392
1	2.867413	0.563092	-3.195131
1	3.336602	2.878860	-3.903505
6	1.137045	-0.261178	-1.295023
6	0.054989	-0.938409	-0.915814
6	0.244780	-2.393873	-0.456103
6	1.515130	-2.919364	-1.176171
6	0.326821	-2.433109	1.078210
1	-0.581739	-2.000665	1.502415
1	0.403356	-3.467144	1.420104
1	1.181707	-1.865960	1.453329
6	2.156999	-4.168845	-0.583252
1	2.977882	-4.517267	-1.215424
1	1.409541	-4.964723	-0.531450
8	-0.790012	-3.265029	-0.908222
1	-1.647861	-2.861866	-0.706430
53	-1.929934	-0.164830	-0.824136
1	1.201631	-3.124265	-2.201488
1	2.552099	-3.995527	0.419553
16	2.699028	-1.510258	-1.297825
1	3.593240	-1.352040	0.629527

S74

8	4.008595	-1.385444	1.546413
8	-4.441008	0.757427	-0.725085
8	6.033254	-0.268037	0.566107
8	5.726702	-0.507022	3.046920
8	-6.882963	0.776741	-0.265120
8	-5.532696	-1.245385	0.270631
16	-5.568471	0.216043	0.081685
16	5.162212	-0.313338	1.728929
8	-5.188696	0.866208	1.597087
8	4.222207	1.016491	1.721113
6	-6.109008	0.550325	2.645278
1	-6.171617	-0.537939	2.761605
1	-7.104724	0.925804	2.382462
6	-5.597268	1.205987	3.917108
1	-5.532573	2.289987	3.792189
1	-6.273538	0.991728	4.751491
1	-4.602893	0.830066	4.171313
6	4.910671	2.301739	1.699328
1	5.572867	2.356639	2.568185
1	5.507081	2.357418	0.785763
6	3.839389	3.370507	1.742042
1	3.245113	3.288141	2.654206
1	4.311030	4.357232	1.722392
1	3.174678	3.286881	0.880530

53

Ph-SO4 RCS=2.2

6	2.235477	-1.114845	-4.593044
6	1.217159	-0.365276	-4.007113
6	0.973374	-0.453629	-2.640255
6	1.745444	-1.305811	-1.830580
6	2.775878	-2.047548	-2.431856
6	3.013960	-1.955474	-3.797995
1	2.423867	-1.041467	-5.658475
1	0.605742	0.292950	-4.614391
1	0.175357	0.126895	-2.198127
1	3.387687	-2.692890	-1.813948
1	3.813651	-2.538034	-4.242031
6	1.479048	-1.420306	-0.405664
6	0.482338	-1.391770	0.458660
6	0.761750	-1.449111	1.972248
6	2.105214	-2.205372	2.171756
6	0.745433	-0.023029	2.542178
1	-0.226461	0.435408	2.346232
1	0.891634	-0.054807	3.623502
1	1.513518	0.605623	2.089413
6	2.732106	-2.060376	3.556790
1	3.593690	-2.725133	3.657937
1	1.997241	-2.339761	4.316215
8	-0.182876	-2.260778	2.669440
1	-1.075744	-1.949200	2.460906
53	-1.571706	-1.147515	-0.114298
1	1.868806	-3.256170	1.994830
1	3.067718	-1.040002	3.752338
16	3.271767	-1.728395	0.831769
1	3.947167	0.240377	1.264246
8	4.333671	1.120604	1.569320
8	-4.117046	-0.811422	-0.775500
8	4.635509	1.744160	-0.846128
8	4.864646	3.434503	0.996688
8	-6.518919	-0.238127	-0.508863
8	-5.019111	-0.264038	1.479113
16	-5.155251	-0.098959	0.021462
16	4.236149	2.247866	0.456940
8	-4.713761	1.505158	-0.284699
8	2.617892	2.426779	0.471036
6	-5.547960	2.494308	0.326142
1	-5.549076	2.351258	1.412925
1	-6.575620	2.379196	-0.036964
6	-4.988479	3.857758	-0.043751
1	-4.984456	3.991086	-1.128672

S75

1	-5.599188	4.650214	0.401479
1	-3.963214	3.965330	0.319602
6	2.030522	3.199159	-0.621889
1	2.518771	4.177278	-0.657765
1	2.220918	2.665670	-1.555289
6	0.551475	3.325343	-0.326121
1	0.385151	3.855834	0.613439
1	0.067883	3.886549	-1.130432
1	0.076252	2.345074	-0.262224

53

Ph-SO4 RCS=2.4

6	2.201774	-1.131947	-4.627988
6	1.227251	-0.320014	-4.050400
6	0.959264	-0.403059	-2.688141
6	1.661571	-1.316162	-1.879624
6	2.647743	-2.123358	-2.471395
6	2.911079	-2.032182	-3.832083
1	2.411013	-1.060797	-5.689652
1	0.670151	0.381980	-4.660793
1	0.192895	0.220340	-2.247117
1	3.207602	-2.806699	-1.845404
1	3.677016	-2.660878	-4.272396
6	1.354823	-1.423305	-0.473873
6	0.421354	-1.384166	0.439063
6	0.724877	-1.410718	1.950427
6	2.045466	-2.206701	2.170468
6	0.757679	0.033472	2.471505
1	-0.201501	0.516062	2.269686
1	0.913787	0.032138	3.551764
1	1.541194	0.620553	1.991320
6	2.613979	-2.091869	3.586027
1	3.442135	-2.791972	3.719397
1	1.835426	-2.340762	4.311739
8	-0.240914	-2.168808	2.676108
1	-1.123282	-1.818439	2.486612
53	-1.652881	-1.128838	-0.120873
1	1.779924	-3.248373	1.980869
1	2.985661	-1.087400	3.798387
16	3.294539	-1.771239	0.895960
1	3.982678	0.149311	1.318294
8	4.390293	1.030642	1.617351
8	-4.169467	-0.795448	-0.735862
8	4.780564	1.592686	-0.799963
8	5.050702	3.304462	1.016166
8	-6.557521	-0.192708	-0.433780
8	-5.017456	-0.186357	1.524538
16	-5.184237	-0.051302	0.067932
16	4.378482	2.136433	0.486568
8	-4.731876	1.536536	-0.286471
8	2.769306	2.401260	0.454914
6	-5.538620	2.551844	0.320551
1	-5.514230	2.434631	1.409984
1	-6.576020	2.441274	-0.014878
6	-4.970535	3.897690	-0.096704
1	-4.992194	4.004604	-1.184273
1	-5.559419	4.708840	0.344043
1	-3.935203	3.999813	0.238351
6	2.261060	3.212260	-0.646405
1	2.805510	4.160932	-0.661641
1	2.445946	2.675456	-1.579317
6	0.783602	3.423574	-0.392095
1	0.622068	3.958097	0.546027
1	0.355787	4.015509	-1.206015
1	0.251972	2.471625	-0.346040

53

Ph-SO4 RCS=2.6

6	2.520276	-3.738296	-3.242965
6	3.047088	-2.459667	-3.048605
6	2.706470	-1.721257	-1.922786

S76

6	1.825904	-2.263854	-0.968709
6	1.312214	-3.561109	-1.161596
6	1.652126	-4.285020	-2.297992
1	2.789047	-4.307831	-4.125987
1	3.729943	-2.035765	-3.776214
1	3.135263	-0.739507	-1.762883
1	0.636557	-3.977413	-0.424897
1	1.240358	-5.277196	-2.444813
6	1.429794	-1.527484	0.189411
6	0.527849	-1.022649	0.964037
6	0.757905	-0.323476	2.318348
6	2.104870	-0.819256	2.930296
6	0.674107	1.194319	2.117215
1	-0.299505	1.458157	1.698002
1	0.773706	1.696690	3.080728
1	1.444494	1.556338	1.437300
6	2.530299	-0.027048	4.171019
1	3.369325	-0.525369	4.661647
1	1.698873	0.025908	4.878926
8	-0.214541	-0.745364	3.275171
1	-1.097410	-0.531909	2.941043
53	-1.525601	-1.044822	0.215251
1	1.909281	-1.850937	3.229217
1	2.845926	0.987262	3.918248
16	3.460579	-0.917290	1.693928
1	3.901496	0.952113	1.090847
8	4.232424	1.906977	0.873096
8	-3.983469	-1.028438	-0.562126
8	4.348015	1.237900	-1.541135
8	4.734406	3.606473	-0.814629
8	-6.414710	-0.556428	-0.450015
8	-4.918716	0.187079	1.399673
16	-5.069350	-0.150595	-0.024724
16	4.060400	2.337815	-0.628650
8	-4.735006	1.273391	-0.861145
8	2.446602	2.577007	-0.618461
6	-5.632549	2.360272	-0.603759
1	-5.617360	2.600037	0.465487
1	-6.651116	2.062552	-0.876572
6	-5.167435	3.542812	-1.436021
1	-5.178491	3.293181	-2.499993
1	-5.827690	4.400967	-1.273245
1	-4.149931	3.831756	-1.161021
6	1.827669	2.925535	-1.893597
1	2.294762	3.842808	-2.262972
1	2.015895	2.114606	-2.601280
6	0.348000	3.113146	-1.633715
1	0.178467	3.914461	-0.911676
1	-0.152251	3.378987	-2.569072
1	-0.106390	2.196243	-1.254929

53

Ph-SO4 RCS=2.8

6	2.716091	-3.723413	-3.248198
6	3.074006	-2.381012	-3.101314
6	2.650386	-1.656966	-1.995925
6	1.857115	-2.281879	-1.012590
6	1.515346	-3.642627	-1.157966
6	1.935874	-4.350595	-2.275771
1	3.049240	-4.280977	-4.116798
1	3.691536	-1.897389	-3.849527
1	2.956712	-0.626647	-1.863253
1	0.908712	-4.118530	-0.397586
1	1.657872	-5.392420	-2.388207
6	1.382043	-1.568046	0.115728
6	0.539417	-1.055756	0.932516
6	0.760365	-0.366501	2.295083
6	2.115322	-0.834752	2.916203
6	0.642025	1.149839	2.105716
1	-0.339016	1.398006	1.694041
1	0.736833	1.644835	3.073349

1	1.401556	1.533829	1.426509
6	2.455518	-0.078743	4.207688
1	3.293927	-0.567003	4.708764
1	1.595938	-0.083535	4.883216
8	-0.211195	-0.822541	3.236815
1	-1.094350	-0.593925	2.914549
53	-1.537890	-1.089657	0.176689
1	1.952732	-1.884746	3.168488
1	2.745814	0.954717	4.007315
16	3.533543	-0.828968	1.748152
1	3.859442	0.994321	1.134677
8	4.160371	1.971120	0.887683
8	-3.966548	-1.080826	-0.553686
8	4.201108	1.296139	-1.526888
8	4.638533	3.660314	-0.820828
8	-6.388973	-0.583357	-0.427367
8	-4.872354	0.159765	1.407293
16	-5.039865	-0.183074	-0.012731
16	3.957515	2.398788	-0.603252
8	-4.693822	1.225785	-0.862450
8	2.344225	2.664520	-0.557331
6	-5.572911	2.329608	-0.606117
1	-5.541446	2.579317	0.460279
1	-6.598363	2.043729	-0.864824
6	-5.098980	3.495495	-1.456145
1	-5.126639	3.235131	-2.517159
1	-5.743898	4.365313	-1.294524
1	-4.074073	3.771302	-1.195912
6	1.718076	3.083355	-1.804318
1	2.186860	4.016598	-2.128860
1	1.894562	2.311812	-2.558279
6	0.240875	3.264196	-1.523656
1	0.081941	4.024105	-0.755763
1	-0.265151	3.585571	-2.438335
1	-0.215839	2.329931	-1.192906

53

Ph-SO4 RCS=3.0

6	2.931352	-3.803807	-3.102913
6	3.186410	-2.433290	-3.008135
6	2.671296	-1.693844	-1.953796
6	1.890763	-2.334540	-0.967798
6	1.652639	-3.723183	-1.060357
6	2.163638	-4.445500	-2.128948
1	3.336042	-4.373048	-3.932706
1	3.796345	-1.939962	-3.756048
1	2.901717	-0.640180	-1.854187
1	1.056346	-4.208154	-0.297502
1	1.968063	-5.509203	-2.202632
6	1.333701	-1.607253	0.103528
6	0.544432	-1.048134	0.927487
6	0.732790	-0.317185	2.273538
6	2.084857	-0.732647	2.943467
6	0.584330	1.189280	2.036592
1	-0.397992	1.406391	1.610451
1	0.662071	1.713384	2.990122
1	1.341840	1.569188	1.353477
6	2.325263	0.033745	4.253520
1	3.155846	-0.425077	4.793423
1	1.434037	-0.001688	4.885582
8	-0.251924	-0.772314	3.202162
1	-1.130856	-0.545655	2.867992
53	-1.546532	-1.114265	0.126849
1	1.953987	-1.788858	3.189117
1	2.590896	1.076295	4.066470
16	3.573796	-0.671122	1.865808
1	3.792889	1.052764	1.199158
8	4.061576	2.055229	0.883744
8	-3.932300	-1.122308	-0.590317
8	4.115973	1.274289	-1.496305
8	4.574129	3.662053	-0.899812

S78

8	-6.354106	-0.641836	-0.450573
8	-4.838003	0.081663	1.394425
16	-5.010534	-0.234240	-0.029904
16	3.882521	2.416984	-0.616848
8	-4.670731	1.184019	-0.857361
8	2.266966	2.707592	-0.606877
6	-5.548316	2.285816	-0.578717
1	-5.507605	2.519866	0.490648
1	-6.575332	2.002918	-0.833730
6	-5.079784	3.462087	-1.416651
1	-5.116776	3.216467	-2.480790
1	-5.722557	4.329894	-1.237447
1	-4.052675	3.733468	-1.161032
6	1.678204	3.127916	-1.867449
1	2.164082	4.054949	-2.184858
1	1.863628	2.353116	-2.616626
6	0.195749	3.325553	-1.625279
1	0.026303	4.089300	-0.863296
1	-0.284838	3.649475	-2.552817
1	-0.278366	2.397220	-1.301887

53

Ph-SO4 RCS=3.2

6	2.602741	-3.625825	-3.474829
6	2.846769	-2.286880	-3.168491
6	2.249492	-1.697288	-2.060918
6	1.404817	-2.478021	-1.242555
6	1.171996	-3.836752	-1.547645
6	1.764685	-4.400475	-2.665555
1	3.070318	-4.073745	-4.345257
1	3.508627	-1.694707	-3.789319
1	2.458440	-0.662970	-1.796405
1	0.522746	-4.421355	-0.907372
1	1.581922	-5.440753	-2.908984
6	0.810618	-1.892961	-0.109923
6	0.210452	-1.330428	0.832078
6	0.393153	-0.728195	2.222932
6	1.530282	-1.464745	3.011854
6	0.629410	0.778838	2.055311
1	-0.182714	1.222446	1.474561
1	0.638522	1.247772	3.040368
1	1.573516	0.991910	1.551566
6	1.782495	-0.813499	4.378342
1	2.423272	-1.464074	4.976262
1	0.839421	-0.662498	4.908322
8	-0.760027	-0.982392	3.023440
1	-1.523434	-0.532432	2.636688
53	-1.883349	-1.049739	-0.145690
1	1.152816	-2.477818	3.170587
1	2.291610	0.146249	4.272990
16	3.110933	-1.750110	2.110020
1	3.425296	-0.459142	1.787390
8	3.878285	1.278496	1.135343
8	-4.115092	-0.692220	-0.797466
8	3.109155	1.166163	-1.223851
8	5.448106	1.833140	-0.726487
8	-6.413808	0.165813	-0.583943
8	-4.804626	0.455354	1.307700
16	-5.033456	0.327021	-0.134050
16	4.057749	1.765897	-0.252284
8	-4.446068	1.712920	-0.832802
8	3.547895	3.357458	-0.084922
6	-5.077383	2.942258	-0.420760
1	-4.966484	3.055451	0.662217
1	-6.144191	2.894175	-0.662333
6	-4.391586	4.069572	-1.169050
1	-4.501205	3.939525	-2.248090
1	-4.837401	5.028287	-0.886842
1	-3.326055	4.099349	-0.931162
6	3.590243	4.148500	-1.280149
1	4.619097	4.183371	-1.655076

S79

1	2.958179	3.683515	-2.044772
6	3.087846	5.537231	-0.924873
1	3.717888	5.989933	-0.155053
1	3.103844	6.180773	-1.810501
1	2.063123	5.492124	-0.547903

53

Ph-SO4 RCS=3.4

6	2.484527	-3.571358	-3.600701
6	2.770672	-2.256260	-3.235143
6	2.188040	-1.695380	-2.104105
6	1.315775	-2.482386	-1.324031
6	1.037199	-3.815706	-1.689077
6	1.617077	-4.350762	-2.828436
1	2.940801	-3.996463	-4.488395
1	3.453537	-1.658896	-3.827705
1	2.424496	-0.678442	-1.798216
1	0.365380	-4.406115	-1.077918
1	1.400554	-5.373053	-3.116580
6	0.749955	-1.924526	-0.157977
6	0.262611	-1.388631	0.851939
6	0.408972	-0.814003	2.250368
6	1.541554	-1.546427	3.054088
6	0.622384	0.700354	2.122880
1	-0.191181	1.145533	1.545351
1	0.614123	1.143840	3.119560
1	1.567412	0.941668	1.633238
6	1.714411	-0.940030	4.453750
1	2.354047	-1.593188	5.050158
1	0.748068	-0.838969	4.952474
8	-0.759775	-1.106964	3.019753
1	-1.518251	-0.651088	2.631021
53	-1.876600	-1.055638	-0.178504
1	1.191043	-2.575919	3.160223
1	2.196995	0.037877	4.405212
16	3.174644	-1.750710	2.219137
1	3.428736	-0.450374	1.893476
8	3.806998	1.315018	1.164581
8	-4.066197	-0.651075	-0.799511
8	3.053512	1.150532	-1.197472
8	5.387499	1.832820	-0.698898
8	-6.334581	0.272508	-0.577188
8	-4.726852	0.473562	1.329295
16	-4.955729	0.389119	-0.114291
16	3.994226	1.771331	-0.231418
8	-4.318176	1.762531	-0.782232
8	3.480229	3.367179	-0.102931
6	-4.888092	3.010079	-0.330298
1	-4.759219	3.088235	0.753448
1	-5.958393	3.016352	-0.560329
6	-4.158718	4.122540	-1.058529
1	-4.287179	4.026298	-2.138939
1	-4.555934	5.092942	-0.745764
1	-3.090447	4.096498	-0.833413
6	3.532500	4.131661	-1.314028
1	4.564142	4.157871	-1.682177
1	2.905856	3.651061	-2.073626
6	3.028893	5.528494	-0.993156
1	3.653492	5.997142	-0.228423
1	3.052305	6.152813	-1.892340
1	2.001303	5.492520	-0.622906

53

Ph-SO4 RCS=3.6

6	2.259015	-3.524203	-3.764252
6	2.623319	-2.248082	-3.336628
6	2.094181	-1.716645	-2.164661
6	1.194883	-2.493588	-1.409395
6	0.832977	-3.784718	-1.837524
6	1.362968	-4.292012	-3.014782
1	2.674228	-3.926279	-4.682298

S80

1	3.325191	-1.656548	-3.912813
1	2.383707	-0.727244	-1.817545
1	0.138299	-4.368831	-1.245967
1	1.082891	-5.284401	-3.349424
6	0.690096	-1.961951	-0.194203
6	0.360757	-1.460139	0.885198
6	0.466739	-0.909172	2.285141
6	1.610408	-1.621682	3.094005
6	0.631619	0.614326	2.200353
1	-0.194679	1.048725	1.633009
1	0.607269	1.029490	3.208757
1	1.568815	0.899112	1.718416
6	1.720161	-1.057364	4.517306
1	2.374671	-1.703265	5.105597
1	0.739461	-1.015902	4.996138
8	-0.707541	-1.260876	3.028172
1	-1.470265	-0.811252	2.641029
53	-1.868682	-1.062302	-0.192203
1	1.301034	-2.667732	3.156192
1	2.161314	-0.058925	4.514859
16	3.275967	-1.729604	2.299647
1	3.452943	-0.422159	1.957224
8	3.738393	1.354943	1.172810
8	-4.015632	-0.609115	-0.762726
8	3.001813	1.110633	-1.188538
8	5.314782	1.865616	-0.695743
8	-6.237697	0.408105	-0.532015
8	-4.627883	0.518543	1.382402
16	-4.860044	0.468945	-0.060558
16	3.920838	1.778514	-0.233855
8	-4.157314	1.811811	-0.712313
8	3.365385	3.365323	-0.148877
6	-4.636055	3.085200	-0.220940
1	-4.478323	3.129297	0.860506
1	-5.708261	3.164242	-0.426828
6	-3.851249	4.162450	-0.943524
1	-4.009982	4.098991	-2.022231
1	-4.176932	5.149226	-0.601145
1	-2.782487	4.061782	-0.743848
6	3.407978	4.099358	-1.378364
1	4.441121	4.140646	-1.741062
1	2.797974	3.585189	-2.129639
6	2.869832	5.491993	-1.097102
1	3.478124	5.994654	-0.340841
1	2.884767	6.093464	-2.011959
1	1.840868	5.441547	-0.732251

53

Ph-SO4 RCS=3.8

6	2.028402	-3.497517	-3.893879
6	2.471616	-2.262692	-3.422201
6	1.997809	-1.752742	-2.216755
6	1.070661	-2.507257	-1.475585
6	0.625207	-3.753367	-1.948678
6	1.104338	-4.242155	-3.156552
1	2.401973	-3.883562	-4.836354
1	3.192633	-1.686001	-3.989938
1	2.342398	-0.792315	-1.840655
1	-0.092437	-4.321241	-1.368674
1	0.760294	-5.202449	-3.523959
6	0.625025	-1.993428	-0.220885
6	0.458153	-1.524180	0.904739
6	0.532680	-0.984010	2.302461
6	1.681402	-1.672536	3.127171
6	0.655097	0.544934	2.242172
1	-0.181605	0.964632	1.679257
1	0.617532	0.944092	3.256515
1	1.584408	0.862251	1.764915
6	1.728898	-1.139403	4.565734
1	2.394138	-1.773461	5.155048
1	0.735678	-1.149103	5.019675



S81

8	-0.647057	-1.380258	3.020630
1	-1.412266	-0.937603	2.630500
53	-1.879430	-1.059892	-0.201531
1	1.410982	-2.730636	3.156135
1	2.130206	-0.124871	4.599440
16	3.376653	-1.697312	2.383124
1	3.486334	-0.391878	2.007978
8	3.699748	1.374046	1.168188
8	-3.994671	-0.557206	-0.718533
8	2.970231	1.054966	-1.187083
8	5.273462	1.850549	-0.711062
8	-6.167378	0.549206	-0.471611
8	-4.552008	0.575016	1.442805
16	-4.790412	0.555473	0.001581
16	3.879443	1.758977	-0.250089
8	-4.029299	1.866292	-0.639770
8	3.305684	3.342439	-0.210058
6	-4.416747	3.157597	-0.110556
1	-4.229419	3.167679	0.966674
1	-5.486767	3.305507	-0.287422
6	-3.584685	4.198417	-0.832914
1	-3.774270	4.167781	-1.907990
1	-3.839839	5.195739	-0.462681
1	-2.519742	4.027956	-0.663063
6	3.344607	4.042226	-1.459058
1	4.378251	4.083634	-1.820416
1	2.741713	3.501725	-2.197592
6	2.792308	5.437030	-1.218362
1	3.393559	5.966526	-0.474874
1	2.803968	6.012877	-2.149641
1	1.762839	5.386850	-0.854785

53

Ph-SO4 RCS=4.0

6	1.909411	-3.484094	-3.970854
6	2.394299	-2.273112	-3.478745
6	1.949394	-1.774373	-2.257364
6	1.007549	-2.514607	-1.522018
6	0.517764	-3.734322	-2.016032
6	0.970227	-4.213870	-3.238610
1	2.261207	-3.861852	-4.924986
1	3.125646	-1.706012	-4.043045
1	2.322466	-0.830373	-1.867608
1	-0.212502	-4.291357	-1.441203
1	0.592357	-5.155495	-3.620990
6	0.591221	-2.010566	-0.247533
6	0.531775	-1.571264	0.900225
6	0.577612	-1.046076	2.301987
6	1.721202	-1.716265	3.153064
6	0.662649	0.486228	2.267276
1	-0.184149	0.894196	1.711043
1	0.615627	0.868123	3.287813
1	1.582858	0.833915	1.793502
6	1.670643	-1.245200	4.613765
1	2.346749	-1.865449	5.205557
1	0.661423	-1.331921	5.020894
8	-0.611553	-1.482334	2.985514
1	-1.375951	-1.047622	2.584847
53	-1.879268	-1.052931	-0.230307
1	1.503890	-2.786413	3.125671
1	2.010243	-0.212219	4.709013
16	3.461153	-1.624591	2.511907
1	3.491806	-0.332411	2.081941
8	3.647253	1.404806	1.165478
8	-3.974544	-0.513510	-0.718856
8	2.939650	1.023037	-1.187666
8	5.234254	1.843619	-0.711412
8	-6.120253	0.634177	-0.449652
8	-4.515147	0.570932	1.473437
16	-4.747458	0.600445	0.032191
16	3.836703	1.754672	-0.260659

S82

8	-3.951409	1.906474	-0.569481
8	3.253824	3.336017	-0.264470
6	-4.287702	3.191716	0.010132
1	-4.092370	3.154594	1.085143
1	-5.352807	3.384328	-0.152563
6	-3.422825	4.226534	-0.681218
1	-3.621074	4.242352	-1.755010
1	-3.638510	5.218183	-0.272763
1	-2.363803	4.011192	-0.526374
6	3.302589	4.005723	-1.529286
1	4.339368	4.041215	-1.882224
1	2.707741	3.446340	-2.260318
6	2.744876	5.404565	-1.327289
1	3.338137	5.953314	-0.591377
1	2.763516	5.957921	-2.272010
1	1.712274	5.360535	-0.971829

53

Ph-SO4 RCS=4.2

6	3.013621	-3.304787	-3.526646
6	3.114299	-1.946345	-3.229052
6	2.471733	-1.419143	-2.114409
6	1.722643	-2.274597	-1.284381
6	1.624709	-3.648538	-1.586265
6	2.268695	-4.156061	-2.704666
1	3.517601	-3.706283	-4.399443
1	3.697926	-1.284198	-3.857527
1	2.567067	-0.367429	-1.874529
1	1.041394	-4.295008	-0.941489
1	2.193340	-5.211946	-2.938583
6	1.081131	-1.760797	-0.129978
6	0.565170	-1.316682	0.901364
6	0.443673	-0.932546	2.356113
6	1.707364	-1.481521	3.133782
6	0.233715	0.578576	2.492266
1	-0.747380	0.848845	2.094508
1	0.274504	0.853482	3.547373
1	0.995553	1.134416	1.945700
6	1.376349	-1.838671	4.589531
1	2.285797	-2.188180	5.085304
1	0.622658	-2.623184	4.637227
8	-0.665843	-1.651956	2.911002
1	-1.470137	-1.377774	2.450086
53	-1.549100	-1.068407	-0.388350
1	2.028890	-2.390267	2.622848
1	1.005553	-0.969617	5.137406
16	3.169438	-0.343129	3.226983
1	3.204573	0.099822	1.937219
8	2.968869	0.843096	0.197000
8	-3.661399	-0.784982	-1.166143
8	3.590115	1.695047	-2.037134
8	4.811694	2.513301	-0.028635
8	-6.038267	-0.182603	-1.047048
8	-4.695051	-0.316613	1.061298
16	-4.752659	-0.044257	-0.374455
16	3.568112	1.956672	-0.580625
8	-4.225971	1.503486	-0.596428
8	2.397345	3.145955	-0.357389
6	-4.985835	2.537835	0.069711
1	-4.975105	2.347505	1.146926
1	-6.020328	2.502956	-0.286344
6	-4.326340	3.860147	-0.269801
1	-4.335327	4.030887	-1.348453
1	-4.866079	4.678072	0.216831
1	-3.290158	3.875088	0.074223
6	2.665904	4.403613	-0.989834
1	3.598065	4.818835	-0.590884
1	2.789509	4.248876	-2.067633
6	1.488758	5.319375	-0.701343
1	1.366503	5.462284	0.375333
1	1.650361	6.297944	-1.165281

S83

1 0.563817 4.894881 -1.099297

53

Ph-SO4 RCS=4.4

6	3.232678	-3.397904	-3.192808
6	3.236269	-2.008920	-3.068764
6	2.463664	-1.392811	-2.094111
6	1.690807	-2.189219	-1.216518
6	1.706876	-3.602470	-1.340702
6	2.466799	-4.195444	-2.331500
1	3.836804	-3.870532	-3.960061
1	3.848394	-1.394692	-3.717593
1	2.500774	-0.316024	-1.981669
1	1.112750	-4.199046	-0.659375
1	2.475926	-5.274000	-2.436933
6	0.933602	-1.590566	-0.210281
6	0.179404	-1.081106	0.656749
6	0.524171	-0.484483	2.031401
6	1.853273	-1.220395	2.423129
6	0.635842	1.032037	1.848264
1	-0.307277	1.422533	1.454045
1	0.833975	1.488615	2.818328
1	1.441478	1.293606	1.161723
6	1.594400	-2.578999	3.078383
1	2.532484	-3.131702	3.156557
1	0.884027	-3.166694	2.491337
8	-0.450892	-0.809463	3.000954
1	-1.247713	-0.290359	2.834776
53	-1.924534	-1.019758	-0.129202
1	2.412922	-1.357601	1.498311
1	1.172459	-2.459559	4.077352
16	2.994162	-0.242330	3.448966
1	3.535409	0.431582	2.404162
8	3.645042	0.548003	0.315506
8	-4.247859	-0.922209	-0.677166
8	3.920096	1.353017	-2.009756
8	5.581238	2.010680	-0.279289
8	-6.614972	-0.276730	-0.444502
8	-4.979420	0.358250	1.334522
16	-5.239839	0.057592	-0.076478
16	4.204101	1.593970	-0.575039
8	-4.826480	1.423774	-0.932660
8	3.226743	2.898266	-0.148148
6	-5.578847	2.610896	-0.618037
1	-5.451227	2.845712	0.443597
1	-6.640400	2.423822	-0.810787
6	-5.046920	3.726029	-1.498841
1	-5.171343	3.476256	-2.555061
1	-5.590045	4.653874	-1.294253
1	-3.985122	3.896487	-1.307217
6	3.515076	4.137612	-0.810329
1	4.548238	4.430197	-0.594193
1	3.413066	4.001754	-1.892858
6	2.530994	5.172428	-0.293294
1	2.633363	5.295707	0.787727
1	2.717005	6.139345	-0.771867
1	1.503073	4.871356	-0.509625

53

Ph-SO4 RCS=4.6

6	2.986351	-3.740873	-3.076131
6	3.078182	-2.350300	-3.029550
6	2.375033	-1.632747	-2.070577
6	1.584601	-2.330759	-1.128993
6	1.511780	-3.745212	-1.171465
6	2.201863	-4.438967	-2.148915
1	3.534628	-4.291543	-3.833179
1	3.704693	-1.813309	-3.731309
1	2.483135	-0.554096	-2.018960
1	0.904943	-4.266026	-0.440925
1	2.141184	-5.520197	-2.192002

S84

6	0.901229	-1.627626	-0.132143
6	0.243492	-1.019599	0.743082
6	0.583024	-0.288359	2.050353
6	1.934416	-0.928675	2.509215
6	0.652494	1.206767	1.725666
1	-0.297408	1.535203	1.293559
1	0.832248	1.754949	2.650782
1	1.457312	1.425040	1.023082
6	1.734738	-2.291335	3.177673
1	2.702377	-2.777694	3.313251
1	1.098405	-2.937815	2.567653
8	-0.379521	-0.552951	3.052271
1	-1.189158	-0.068189	2.849250
53	-1.903040	-1.031578	-0.029067
1	2.550212	-1.025418	1.616635
1	1.255208	-2.185047	4.151990
16	2.937374	0.145352	3.605324
1	3.566616	0.780376	2.589907
8	3.727263	0.552871	0.335377
8	-4.213266	-0.965398	-0.516531
8	3.791222	1.124765	-2.075949
8	5.577017	1.969227	-0.567101
8	-6.557996	-0.239718	-0.319760
8	-4.874565	0.554113	1.348930
16	-5.171432	0.105214	-0.013723
16	4.188732	1.506683	-0.698881
8	-4.740888	1.349907	-1.026848
8	3.224169	2.839816	-0.324853
6	-5.447919	2.590831	-0.832047
1	-5.283864	2.939172	0.192552
1	-6.519365	2.418514	-0.977566
6	-4.905332	3.579507	-1.846761
1	-5.066629	3.216233	-2.864287
1	-5.413241	4.542525	-1.736348
1	-3.833953	3.734053	-1.700823
6	3.436844	4.008973	-1.127153
1	4.478141	4.332870	-1.023936
1	3.253698	3.764378	-2.179546
6	2.477388	5.080678	-0.639317
1	2.660483	5.312152	0.412957
1	2.608964	5.996904	-1.224005
1	1.441158	4.749765	-0.743601

53

Ph-SO4 RCS=4.8

6	2.732466	-4.085157	-2.943429
6	2.953653	-2.708718	-2.934347
6	2.331406	-1.901123	-1.989244
6	1.490215	-2.497333	-1.024648
6	1.284414	-3.896361	-1.026603
6	1.896585	-4.679143	-1.990361
1	3.216827	-4.704627	-3.690783
1	3.616880	-2.252171	-3.659290
1	2.536011	-0.833352	-1.967617
1	0.637530	-4.339125	-0.279012
1	1.732407	-5.750457	-2.001988
6	0.890510	-1.697429	-0.037095
6	0.350201	-0.989520	0.835083
6	0.644073	-0.143800	2.076645
6	2.025242	-0.653997	2.601739
6	0.638901	1.324906	1.641842
1	-0.322689	1.574333	1.184377
1	0.784924	1.946164	2.525631
1	1.437277	1.532570	0.928275
6	1.920085	-2.015281	3.293804
1	2.920630	-2.401051	3.496207
1	1.389591	-2.735209	2.664860
8	-0.314283	-0.387344	3.091692
1	-1.144542	0.042033	2.851197
53	-1.842937	-1.054877	0.024876
1	2.688068	-0.703414	1.739623

S85

1	1.375968	-1.937268	4.236529
16	2.866194	0.533924	3.739144
1	3.544120	1.166310	2.755462
8	3.848182	0.717732	0.427942
8	-4.120144	-0.985526	-0.442857
8	3.696975	0.885768	-2.043261
8	5.501207	2.096831	-0.839645
8	-6.447064	-0.209185	-0.263781
8	-4.738064	0.626836	1.360137
16	-5.055935	0.130092	0.020239
16	4.152931	1.515391	-0.779045
8	-4.605923	1.314989	-1.048147
8	3.102683	2.819514	-0.549804
6	-5.275641	2.584713	-0.899525
1	-5.086872	2.971853	0.106454
1	-6.353124	2.436044	-1.023914
6	-4.718946	3.510427	-1.964218
1	-4.904886	3.107360	-2.962279
1	-5.197732	4.491561	-1.890246
1	-3.641837	3.640264	-1.838631
6	3.162430	3.849835	-1.544350
1	4.177026	4.261567	-1.576955
1	2.932686	3.420340	-2.526104
6	2.149686	4.915915	-1.163030
1	2.380447	5.332669	-0.179385
1	2.165387	5.728648	-1.896481
1	1.140277	4.498379	-1.131532

53

Ph-SO4 RCS=5.0

6	1.909365	-4.627204	-2.542204
6	2.363496	-3.311122	-2.618461
6	1.885554	-2.348510	-1.735779
6	0.953231	-2.727147	-0.748173
6	0.507370	-4.061338	-0.663047
6	0.980217	-5.001080	-1.566092
1	2.282517	-5.368925	-3.240245
1	3.097377	-3.026961	-3.363464
1	2.249176	-1.323960	-1.757029
1	-0.210837	-4.337210	0.099585
1	0.632076	-6.026126	-1.510101
6	0.518968	-1.748536	0.176453
6	0.216689	-0.846414	0.971788
6	0.590674	0.217033	1.996033
6	1.954703	-0.227172	2.617928
6	0.668073	1.550869	1.243711
1	-0.305428	1.788246	0.805294
1	0.944704	2.332504	1.950741
1	1.410331	1.496956	0.444296
6	1.826313	-1.491608	3.471000
1	2.818383	-1.824822	3.778828
1	1.348395	-2.299859	2.909916
8	-0.354793	0.259532	3.053465
1	-1.164191	0.677396	2.735200
53	-2.078639	-0.887774	0.213840
1	2.652008	-0.383012	1.795066
1	1.227502	-1.303541	4.363802
16	2.753299	1.114939	3.628232
1	3.669401	1.416306	2.678716
8	4.550403	0.654838	0.783798
8	-4.327082	-0.690040	-0.173250
8	2.983461	0.527328	-1.136083
8	5.416244	0.254843	-1.526834
8	-6.541153	0.373807	-0.153756
8	-4.679511	1.376419	1.185473
16	-5.112695	0.614196	0.014716
16	4.365959	0.827236	-0.668811
8	-4.580261	1.434750	-1.319292
8	4.509477	2.495931	-0.819706
6	-5.067928	2.786744	-1.466882
1	-4.770189	3.369555	-0.590248

S86

1	-6.160972	2.766314	-1.523740
6	-4.457991	3.343427	-2.738712
1	-4.754946	2.746116	-3.603634
1	-4.797616	4.372029	-2.892866
1	-3.367701	3.344357	-2.675896
6	4.425869	3.009898	-2.154747
1	5.228188	2.575829	-2.761222
1	3.464774	2.721836	-2.595819
6	4.556588	4.520967	-2.070189
1	5.512977	4.800115	-1.620888
1	4.501091	4.960389	-3.071524
1	3.754380	4.944452	-1.460768

53

Ph-SO4 RCS=5.2

6	1.578194	-4.965377	-2.057874
6	2.280580	-3.761378	-2.088700
6	1.869898	-2.682565	-1.311178
6	0.742278	-2.827280	-0.481154
6	0.036913	-4.041370	-0.446120
6	0.456143	-5.102935	-1.237342
1	1.902593	-5.798456	-2.672127
1	3.155571	-3.653109	-2.719274
1	2.411755	-1.739890	-1.314992
1	-0.835144	-4.138154	0.189122
1	-0.091405	-6.038418	-1.215103
6	0.384819	-1.716116	0.343140
6	0.339585	-0.710160	1.059327
6	0.681718	0.496489	1.907282
6	2.070326	0.215351	2.579792
6	0.707553	1.716758	0.977779
1	-0.273410	1.858705	0.515886
1	0.959856	2.596871	1.568595
1	1.454412	1.573292	0.194231
6	2.016375	-0.957035	3.561005
1	3.022380	-1.176824	3.920567
1	1.619263	-1.854895	3.077329
8	-0.260731	0.649814	2.962669
1	-1.090770	0.978567	2.596569
53	-2.102543	-0.857647	0.318759
1	2.782095	0.016221	1.779767
1	1.381051	-0.725313	4.417645
16	2.773095	1.721469	3.446348
1	3.751195	1.898283	2.527192
8	4.798416	0.972766	0.802956
8	-4.320799	-0.652250	-0.019467
8	3.154584	0.183034	-0.878369
8	5.579765	-0.005627	-1.361929
8	-6.500027	0.473298	-0.080304
8	-4.576260	1.576033	1.084495
16	-5.064428	0.696822	0.024256
16	4.526493	0.706310	-0.620654
8	-4.540955	1.325097	-1.409262
8	4.504453	2.267859	-1.247751
6	-4.976786	2.671652	-1.709539
1	-4.627250	3.341461	-0.918723
1	-6.070827	2.692635	-1.734917
6	-4.384034	3.040012	-3.055362
1	-4.732908	2.356114	-3.832172
1	-4.685024	4.056484	-3.325666
1	-3.293292	2.999516	-3.021261
6	4.326016	2.367193	-2.665697
1	5.140099	1.837195	-3.171823
1	3.378281	1.893921	-2.947744
6	4.325445	3.843725	-3.022991
1	5.269917	4.310251	-2.731814
1	4.193050	3.970146	-4.102516
1	3.512983	4.365082	-2.510700

53

Ph-SO4 RCS=5.4

S87

6	1.434333	-5.221331	-1.363355
6	2.252929	-4.093231	-1.411509
6	1.860300	-2.906306	-0.800141
6	0.627139	-2.858918	-0.123734
6	-0.198272	-3.991367	-0.077774
6	0.209322	-5.167553	-0.696841
1	1.747371	-6.140738	-1.846314
1	3.204973	-4.128368	-1.928805
1	2.487380	-2.018944	-0.834501
1	-1.151504	-3.942922	0.433993
1	-0.431160	-6.041669	-0.661129
6	0.287775	-1.623718	0.532272
6	0.446690	-0.539232	1.117027
6	0.760352	0.809722	1.752610
6	2.148377	0.734372	2.496541
6	0.763366	1.853594	0.627757
1	-0.212433	1.884986	0.135490
1	0.980285	2.828807	1.063444
1	1.528733	1.600657	-0.108246
6	2.128869	-0.272620	3.645889
1	3.131318	-0.370785	4.064103
1	1.806037	-1.257169	3.291018
8	-0.209595	1.104555	2.753728
1	-1.046648	1.325282	2.326980
53	-2.119235	-0.807986	0.449083
1	2.896909	0.459308	1.756046
1	1.446842	0.041326	4.438080
16	2.764885	2.413100	3.148190
1	3.766033	2.477550	2.240092
8	4.880681	1.246855	0.668919
8	-4.338554	-0.617748	0.156267
8	3.282130	-0.052677	-0.710722
8	5.714706	-0.238117	-1.163318
8	-6.499059	0.530880	-0.020828
8	-4.513280	1.771581	0.870199
16	-5.057568	0.737307	-0.006504
16	4.624709	0.590752	-0.625220
8	-4.578291	1.098277	-1.543191
8	4.516084	1.920807	-1.652089
6	-5.003192	2.383457	-2.055648
1	-4.612024	3.170650	-1.404938
1	-6.096838	2.424591	-2.045289
6	-4.457324	2.501535	-3.464924
1	-4.846922	1.702308	-4.099179
1	-4.752555	3.462869	-3.895599
1	-3.366848	2.443509	-3.463168
6	4.341114	1.621829	-3.042050
1	5.186867	1.021003	-3.393362
1	3.423430	1.037297	-3.176647
6	4.258930	2.943621	-3.786368
1	5.173565	3.524047	-3.641458
1	4.126382	2.764772	-4.858435
1	3.414996	3.537921	-3.427251