

2,4,6-trihydroxyacetophenone , CNDO/S-CI calculation

1 2,4,6-trihydroxyacetophenone 05-M

ADJUSTED OPTION CARD IMAGE

```

-----NOPT-----
N  NA  NOCC NITER NCONF  1  2  3  4  5  6  7  9  10  11  12  13  14  15
56, 20, 32, 40, 60, 1, 2, 2, 1, 3, 0, 1, 1, 0, 0, 0, 0,
0, 0,
    
```

ADJUSTED PARAMETER CARD IMAGE

```

TCONV      ENGM      EMAX      FKAP
0.000010  9.000000  9.000000  0.000000
    
```

```

-----COORDINATES----- AT.
ATOM      X      Y      Z      NO.      USS      UPP      S      P
-----BETAO-----
1  1.47550  1.45790  0.04750  6  29.920000  11.610000 -17.500000 -17.500000
2  -0.05620  1.48460  0.04790  6  29.920000  11.610000 -17.500000 -17.500000
3  -0.81850  0.14420  0.03110  6  29.920000  11.610000 -17.500000 -17.500000
4  -0.05100 -1.19230  0.01420  6  29.920000  11.610000 -17.500000 -17.500000
5  1.48220 -1.14360  0.01470  6  29.920000  11.610000 -17.500000 -17.500000
6  2.28060  0.15930  0.03110  6  29.920000  11.610000 -17.500000 -17.500000
7  -2.37710  0.14420  0.03110  6  29.920000  11.610000 -17.500000 -17.500000
8  -3.15420  1.29360  0.04630  8  54.509998  21.930000 -45.000000 -45.000000
9  -0.77060  2.86370  0.06530  8  54.509998  21.930000 -45.000000 -45.000000
10  3.83000  0.16090  0.03100  8  54.509998  21.930000 -45.000000 -45.000000
11  -0.72970 -2.59260 -0.00330  8  54.509998  21.930000 -45.000000 -45.000000
12  -3.08520 -1.23350  0.01270  6  29.920000  11.610000 -17.500000 -17.500000
13  -1.87450  2.71760  0.06400  1  14.350000 -12.000000
14  4.21110 -0.87910  0.01810  1  14.350000 -12.000000
15  2.02100  2.41300  0.05940  1  14.350000 -12.000000
16  2.03830 -2.09260  0.00280  1  14.350000 -12.000000
17  0.02120 -3.52640 -0.01520  1  14.350000 -12.000000
18  -2.33100 -2.04780  0.00180  1  14.350000 -12.000000
19  -3.72260 -1.32070 -0.89170  1  14.350000 -12.000000
20  -3.72260 -1.34480  0.91450  1  14.350000 -12.000000
    
```

COORDINATES FROM

2,4,6-trihydroxyacetophenone

BETA ZEROS FROM DELBENE/JAFFE, WITH KAPPA = 0.585

MATAGA INTEGRALS USED

THE POINT GROUP OF THE MOLECULE IS CS

```

COORDINATES IN      PRINCIPAL      AXIS SYSTEM
ATOM      X      Y      Z      AT.=
1  -1.34640  1.65350 -0.00010  6
2  -1.37001  0.12175 -0.00008  6
3  -0.02797 -0.63784  0.00009  6
4  1.30709  0.13235  0.00015  6
5  1.25529  1.66545  0.00007  6
6  -0.04932  2.46122 -0.00002  6
7  -0.02482 -2.19644  0.00004  6
8  -1.17275 -2.97586  0.00066  8
9  -2.74777 -0.59543 -0.00018  8
10 -0.05404  4.01061 -0.00010  8
11  2.70886 -0.54352  0.00037  8
12  1.35442 -2.90176 -0.00091  6
13  -2.59944 -1.69903  0.00034  1
14  0.98527  4.39381  0.00019  1
15  -2.30267  2.19707 -0.00029  1
16  2.20324  2.22346  0.00021  1
17  3.64122  0.20926  0.00033  1
18  2.16727 -2.14592 -0.00147  1
19  1.45436 -3.53894 -0.90415  1
20  1.45557 -3.53898  0.90221  1
    
```

1 part e ch eton ica nari ngin a

05-M



SEVERAL ATOMS SUPERIMPOSED. SYMBOL AND NUMBER REFER TO THE HIGHEST NUMBERED

PROJECTION ON THE X-Y PLANE  
1 2,4,6-trihydroxyacetophenone 05-M  
THE NUCLEAR REPULSION ENERGY CALCULATED BY GAMMAS IS 6231.81494EV

THE ELECTRONIC ENERGY AFTER	1	ITERATIONS IS	-9179.73242
THE ELECTRONIC ENERGY AFTER	2	ITERATIONS IS	-9168.68457
THE ELECTRONIC ENERGY AFTER	3	ITERATIONS IS	-9214.89551
THE ELECTRONIC ENERGY AFTER	4	ITERATIONS IS	-9196.88770
THE ELECTRONIC ENERGY AFTER	5	ITERATIONS IS	-9209.19141

DENSITY MATRIX AVERAGING BEGUN

THE ELECTRONIC ENERGY AFTER	6	ITERATIONS IS	-9204.48145
THE ELECTRONIC ENERGY AFTER	7	ITERATIONS IS	-9204.14941
THE ELECTRONIC ENERGY AFTER	8	ITERATIONS IS	-9204.06641

ITERATION CONTINUES AFTER CONVERGENCE OF ENERGY BECAUSE OF NON-CONVERGENCE OF DENSITY MATRIX

THE ELECTRONIC ENERGY AFTER	9	ITERATIONS IS	-9204.01074
-----------------------------	---	---------------	-------------

ITERATION CONTINUES AFTER CONVERGENCE OF ENERGY BECAUSE OF NON-CONVERGENCE OF DENSITY MATRIX

THE ELECTRONIC ENERGY AFTER	10	ITERATIONS IS	-9204.01563
-----------------------------	----	---------------	-------------

ITERATION CONTINUES AFTER CONVERGENCE OF ENERGY BECAUSE OF NON-CONVERGENCE OF DENSITY MATRIX

THE ELECTRONIC ENERGY AFTER	11	ITERATIONS IS	-9203.99902
-----------------------------	----	---------------	-------------

ITERATION CONTINUES AFTER CONVERGENCE OF ENERGY BECAUSE OF NON-CONVERGENCE OF DENSITY MATRIX

THE ELECTRONIC ENERGY AFTER	12	ITERATIONS IS	-9203.99805
-----------------------------	----	---------------	-------------

ITERATION CONTINUES AFTER CONVERGENCE OF ENERGY BECAUSE OF NON-CONVERGENCE OF DENSITY MATRIX

THE ELECTRONIC ENERGY AFTER	13	ITERATIONS IS	-9203.99414
-----------------------------	----	---------------	-------------

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

AFTER 13 ITERATIONS THE ELECTRONIC ENERGY HAS CONVERGED TO A RELATIVE PRECISION OF 0.000000424  
 AND THE DENSITY MATRIX TO LESS THAN 0.0010000

THE ELECTRONIC ENERGY IS -9203.99219 EV AND THE TOTAL ENERGY IS -2972.17725 EV

1	2,4,6-trihydroxyacetophenone		05-M					
	ATOM	ATOM	ELECTRONIC	REPULSION	INTEGRALS	ELECTRON DENSITIES	CHARGE DENSITIES	INTERATOM.DIST.
	1	1	10.930000			4.038797	-0.038797	
	2	1	5.052739					1.53193
	2	2	10.930000			3.826221	0.173779	
	3	1	3.634553					2.64358
	3	2	5.034780					1.54209
	3	3	10.930000			4.016814	-0.016814	
	4	1	3.289842					3.05857
	4	2	3.604035					2.67712
	4	3	5.036198					1.54129
	4	4	10.930000			3.860471	0.139529	
	5	1	3.673382					2.60172
	5	2	3.299683					3.04552
	5	3	3.640924					2.63665
	5	4	5.049122					1.53397
	5	5	10.930000			4.062149	-0.062149	
	6	1	5.059704					1.52801
	6	2	3.595579					2.68651
	6	3	3.259624					3.09914
	6	4	3.587897					2.69508
	6	5	5.059446					1.52816
	6	6	10.930000			3.854272	0.145728	
	7	1	2.671939					4.07046
	7	2	3.601245					2.68021
	7	3	5.005881					1.55860
	7	4	3.598941					2.68277
	7	5	2.672897					4.06852
	7	6	2.409309					4.65772
	7	7	10.930000			3.704131	0.295869	
	8	1	2.508988					4.63262
	8	2	3.420344					3.10388
	8	3	3.882151					2.60324
	8	4	2.833098					3.97625
	8	5	2.269500					5.23805
	8	6	2.162487					5.55193
	8	7	5.775819					1.38753
	8	8	15.130000			6.508785	-0.508785	
	9	1	3.833984					2.64982
	9	2	5.415709					1.55325
	9	3	3.763502					2.72014
	9	4	2.755333					4.11966
	9	5	2.524481					4.59740
	9	6	2.777828					4.07735
	9	7	3.376329					3.15875
	9	8	3.782447					2.85432
	9	9	15.130000			6.320203	-0.320203	
	10	1	3.795241					2.68815
	10	2	2.762826					4.10549
	10	3	2.502048					4.64853
	10	4	2.760339					4.11018
	10	5	3.797477					2.68592
	10	6	5.423563					1.54940
	10	7	1.968714					6.20712
	10	8	1.793347					7.07547
	10	9	2.289529					5.33590
	10	10	15.130000			6.299096	-0.299096	
	11	1	2.517964					4.61216
	11	2	2.748434					4.13277
	11	3	3.745562					2.73846
	11	4	5.409691					1.55621
	11	5	3.839611					2.64432
	11	6	2.777087					4.07873
	11	7	3.348209					3.19456
	11	8	2.602056					4.58074
	11	9	2.246304					5.45688
	11	10	2.292881					5.32671
	11	11	15.130000			6.296190	-0.296190	
	12	1	2.176854					5.29574
	12	2	2.672211					4.06991
	12	3	3.626288					2.65261
	12	4	3.308057					3.03448
	12	5	2.445924					4.56828
	12	6	2.098193					5.54365
	12	7	5.022423					1.54913
	12	8	3.962265					2.52827
	12	9	2.477268					4.70608
	12	10	1.764273					7.05441

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

12	11	3.764109			2.71952
12	12	10.930000	4.075250	-0.075250	
13	1	3.005387			3.57905
13	2	4.224293			2.19699
13	3	3.605496			2.78184
13	4	2.605342			4.31450
13	5	2.275099			5.11652
13	6	2.363589			4.87963
13	7	3.755634			2.62223
13	8	4.890342			1.91461
13	9	6.718862			1.11353
13	10	1.977259			6.25133
13	11	2.227788			5.43262
13	12	2.693962			4.13275
13	13	12.850000	0.785348	0.214652	
14	1	2.993515			3.59805
14	2	2.364106			4.87830
14	3	2.269309			5.13266
14	4	2.624777			4.27359
14	5	3.642117			2.74169
14	6	4.230371			2.19209
14	7	1.827266			6.66721
14	8	1.653062			7.67913
14	9	1.982736			6.23122
14	10	6.737178			1.10770
14	11	2.300077			5.22954
14	12	1.690430			7.30490
14	13	1.757764			7.06915
14	14	12.850000	0.812925	0.187075	
15	1	6.229853			1.09997
15	2	4.129442			2.27526
15	3	2.970873			3.63470
15	4	2.681025			4.15854
15	5	2.993881			3.59746
15	6	4.137136			2.26878
15	7	2.337013			4.94889
15	8	2.276305			5.29490
15	9	3.732462			2.82775
15	10	3.674291			2.88881
15	11	2.135473			5.71194
15	12	1.923070			6.27474
15	13	2.863180			3.90739
15	14	2.836737			3.95426
15	15	12.850000	0.943004	0.056996	
16	1	2.995347			3.59511
16	2	2.687540			4.14552
16	3	2.974730			3.62841
16	4	4.129695			2.27505
16	5	6.229777			1.10000
16	6	4.141545			2.26507
16	7	2.336694			4.94973
16	8	1.991515			6.19922
16	9	2.140137			5.69726
16	10	3.683419			2.87911
16	11	3.746988			2.81280
16	12	2.247211			5.19504
16	13	1.966212			6.20095
16	14	3.988658			2.48875
16	15	2.558555			4.50599
16	16	12.850000	0.959857	0.040143	
17	1	2.248098			5.19251
17	2	2.313313			5.01200
17	3	2.892660			3.76571
17	4	4.059409			2.33540
17	5	3.593465			2.79520
17	6	2.601175			4.32336
17	7	2.572569			4.38489
17	8	2.116526			5.77229
17	9	1.927449			6.43947
17	10	2.273952			5.30144
17	11	6.463066			1.19832
17	12	2.838268			3.86107
17	13	1.882649			6.52591
17	14	2.368963			4.95627
17	15	1.948507			6.26747
17	16	4.004098			2.47483
17	17	12.850000	0.809685	0.190315	
18	1	2.254234			5.17508
18	2	2.659619			4.20175
18	3	3.715778			2.66334
18	4	3.948239			2.43525
18	5	2.806240			3.91896
18	6	2.276497			5.11263
18	7	4.229641			2.19268
18	8	3.219964			3.44160
18	9	2.328250			5.15381
18	10	1.900592			6.54501
18	11	5.291508			1.69145
18	12	6.203015			1.10996
18	13	2.436588			4.78762

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

1	SYMM	EIGENVALUE	ATOM ORB	EIGENVECTOR	ORBITALS	DENS. MAT.	BETAS
18		14		1.853611			6.64569
18		15		1.957820			6.23233
18		16		2.622153			4.36953
18		17		3.692339			2.77838
18		18		12.850000	0.916083	0.083917	
19		1		2.005104			5.96850
19		2		2.430831			4.71116
19		3		3.135005			3.38102
19		4		2.882133			3.78389
19		5		2.215712			5.28610
19		6		1.929079			6.25143
19		7		4.229638			2.19268
19		8		3.725419			2.83505
19		9		2.307448			5.20954
19		10		1.639407			7.75166
19		11		3.271541			3.37112
19		12		6.203255			1.10987
19		13		2.541940			4.54276
19		14		1.578723			7.99790
19		15		1.791214			6.91622
19		16		2.056122			5.88081
19		17		2.592294			4.43276
19		18		4.918395			1.80653
19		19		12.850000	0.955367	0.044633	
20		1		2.005008			5.96884
20		2		2.430660			4.71158
20		3		3.135002			3.38102
20		4		2.882387			3.78344
20		5		2.215802			5.28584
20		6		1.929063			6.25149
20		7		4.229630			2.19269
20		8		3.725330			2.83514
20		9		2.307180			5.21027
20		10		1.639393			7.75174
20		11		3.272382			3.36999
20		12		6.203150			1.10991
20		13		2.541683			4.54334
20		14		1.578748			7.99775
20		15		1.791099			6.91673
20		16		2.056261			5.88034
20		17		2.592801			4.43168
20		18		4.918296			1.80659
20		19		4.918687			1.80636
20		20		12.850000	0.955361	0.044639	
1		2,4,6-trihydroxyacetophenone		05-M			
	OVERLAP						
1	A*	-43.680347	1 S	-0.12115840	1 1	1.09143	0.00000
1.00000			X	-0.01688005	1 2	-0.04430	0.00000
0.00000			Y	0.04051343	1 3	0.01781	0.00000
0.00000			Z	-0.00000186	1 4	0.00003	0.00000
0.00000			2 S	-0.26617843	1 5	0.31263	-6.02048
0.34403			X	0.03947026	1 6	-0.01788	-0.09923
0.00567			Y	0.06895040	1 7	0.48646	-6.43682
0.36782			Z	-0.00000343	1 8	0.00001	0.00008
0.00000			3 S	-0.27308142	1 9	-0.01125	-1.01384
0.05793			X	0.00492060	1 10	0.02177	0.67796
0.03874			Y	0.03237606	1 11	-0.01426	-1.17825
0.06733			Z	0.00000560	1 12	0.00000	0.00010
0.00001			4 S	-0.28249273	1 13	-0.01476	-0.45881
0.02622			X	-0.05718126	1 14	-0.00081	0.55587
0.03176			Y	0.05760411	1 15	0.00004	-0.31866
0.01821			Z	-0.00000546	1 16	-0.00002	0.00005
0.00000			5 S	-0.13968994	1 17	-0.01006	-1.09480
0.06256			X	0.00947460	1 18	0.01851	1.46076
0.08347			Y	0.04429625	1 19	-0.01090	0.00671
0.00038			Z	-0.00000274	1 20	-0.00001	0.00010
0.00001							

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.34580		6	S	-0.11901852	1	21	0.31473	-6.05141	
			X	-0.00495126	1	22	-0.42631	5.48513	-
0.31344			Y	0.00763246	1	23	-0.21915	3.41571	-
0.19518			Z	0.00000013	1	24	0.00000	0.00034	-
0.00002		7	S	-0.35157886	1	25	0.02398	-0.05494	
0.00314			X	0.06793240	1	26	-0.00864	0.02650	-
0.00151			Y	0.02229398	1	27	0.03346	-0.07719	
0.00441			Z	-0.00002556	1	28	0.00002	0.00000	
0.00000		8	S	-0.33703706	1	29	-0.00137	-0.00541	
0.00017			X	-0.06855121	1	30	0.00689	0.00026	-
0.00001			Y	-0.07513454	1	31	-0.00493	-0.00702	
0.00022			Z	0.00005027	1	32	-0.00002	0.00000	
0.00000		9	S	-0.36486340	1	33	-0.01758	-0.76013	
0.02432			X	-0.06967694	1	34	-0.01878	-0.46788	
0.01497			Y	0.02186608	1	35	-0.03447	-0.75085	
0.02403			Z	-0.00002649	1	36	-0.00002	-0.00003	
0.00000		10	S	-0.10873829	1	37	-0.01762	-0.69698	
0.02230			X	-0.01015973	1	38	0.01790	0.39154	-
0.01253			Y	0.01920801	1	39	0.03136	0.71413	-
0.02285			Z	-0.00000368	1	40	-0.00001	0.00000	
0.00000		11	S	-0.40383106	1	41	0.00151	-0.00571	
0.00018			X	0.05854595	1	42	-0.00297	0.00652	-
0.00021			Y	-0.01569272	1	43	-0.00174	-0.00353	
0.00011			Z	0.00003751	1	44	0.00000	0.00000	
0.00000		12	S	-0.20181946	1	45	-0.00820	-0.00328	
0.00019			X	0.04129513	1	46	0.01100	0.00259	-
0.00015			Y	-0.05257551	1	47	-0.00889	-0.00437	
0.00025			Z	-0.00003862	1	48	-0.00001	0.00000	
0.00000		13	S	-0.18923205	1	49	0.03775	-0.13654	
0.00926		14	S	-0.04701435	1	50	0.03817	-0.13163	
0.00892		15	S	-0.04228612	1	51	0.56042	-7.57130	
0.51331		16	S	-0.05535062	1	52	0.04103	-0.13238	
0.00897		17	S	-0.13169251	1	53	0.00007	-0.00529	
0.00036		18	S	-0.14411065	1	54	-0.00112	-0.00548	
0.00037		19	S	-0.07756725	1	55	0.00415	-0.00103	
0.00007		20	S	-0.07757101	1	56	0.00415	-0.00103	
0.00007									
2	A*	-42.368504	1	S	-0.02122656	2	1	-0.04430	0.00000
0.00000			X	-0.05323897	2	2	0.95436	0.00000	
1.00000			Y	-0.06441319	2	3	-0.03735	0.00000	
0.00000			Z	-0.00000181	2	4	-0.00002	0.00000	
0.00000		2	S	0.18314715	2	5	0.00407	0.09923	-
0.00567			X	-0.11616777	2	6	0.07510	-1.99099	
0.11377			Y	-0.09220794	2	7	0.00603	0.11962	-
0.00684			Z	-0.00000105	2	8	-0.00007	0.00000	
0.00000									

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.03874	3	S	0.01564713	2	9	-0.00431	-0.67796	
		X	-0.11039370	2	10	0.00077	0.27619	-
0.01578		Y	-0.04231177	2	11	0.02087	-0.85729	
0.04899		Z	0.00000108	2	12	0.00000	0.00007	
0.00000	4	S	-0.24832200	2	13	-0.00006	-0.55587	
0.03176		X	-0.12120485	2	14	-0.01359	0.63870	-
0.03650		Y	0.02905602	2	15	0.00794	-0.41550	
0.02374		Z	-0.00001318	2	16	0.00003	0.00007	
0.00000	5	S	-0.17418413	2	17	-0.02160	-1.46076	
0.08347		X	0.00330279	2	18	0.00276	1.88554	-
0.10775		Y	0.01121727	2	19	-0.02827	0.00975	-
0.00056		Z	-0.00000352	2	20	0.00000	0.00014	-
0.00001	6	S	-0.21859844	2	21	0.43498	-5.48513	
0.31344		X	-0.02720505	2	22	-0.45606	3.59983	-
0.20570		Y	-0.09548168	2	23	-0.28127	3.49125	-
0.19950		Z	0.00000220	2	24	-0.00011	0.00035	-
0.00002	7	S	0.13583438	2	25	0.00709	-0.02650	
0.00151		X	-0.13261075	2	26	0.00043	0.00563	-
0.00032		Y	-0.04974379	2	27	0.00554	-0.03933	
0.00225		Z	0.00005294	2	28	0.00001	0.00000	
0.00000	8	S	0.26081735	2	29	0.00001	-0.00034	
0.00001		X	0.03086571	2	30	-0.00095	-0.00054	
0.00002		Y	0.05866364	2	31	-0.00049	-0.00046	
0.00001		Z	-0.00003223	2	32	0.00000	0.00000	
0.00000	9	S	0.41496590	2	33	0.00736	0.62767	-
0.02009		X	0.06729373	2	34	0.00315	0.28322	-
0.00906		Y	-0.02416635	2	35	-0.01222	0.67013	-
0.02144		Z	0.00002813	2	36	0.00002	0.00002	
0.00000	10	S	-0.37825105	2	37	-0.01050	-0.52451	
0.01678		X	-0.03686711	2	38	0.00491	0.19658	-
0.00629		Y	0.05058484	2	39	0.04029	0.58022	-
0.01857		Z	-0.00001270	2	40	0.00001	0.00000	
0.00000	11	S	-0.45288530	2	41	0.00177	-0.00838	
0.00027		X	0.04869363	2	42	-0.00283	0.00940	-
0.00030		Y	-0.03656875	2	43	-0.00321	-0.00541	
0.00017		Z	0.00002890	2	44	-0.00001	0.00000	
0.00000	12	S	-0.03236388	2	45	-0.00162	-0.00259	
0.00015		X	-0.04841300	2	46	0.00049	0.00177	-
0.00010		Y	-0.03265938	2	47	-0.00050	-0.00359	
0.00021		Z	0.00001369	2	48	0.00000	0.00000	
0.00000	13	S	0.20206945	2	49	-0.00590	0.06431	-
0.00436	14	S	-0.16243267	2	50	0.03031	-0.11485	
0.00779	15	S	-0.00281192	2	51	-0.71098	6.22548	-
0.42207	16	S	-0.08524513	2	52	0.04538	-0.17596	
0.01193	17	S	-0.15974140	2	53	0.00057	-0.00712	
0.00048								

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00035		18	S	-0.09428903	2	54	0.00076	-0.00522	
		19	S	-0.00648012	2	55	0.00064	-0.00069	
0.00005		20	S	-0.00649448	2	56	0.00063	-0.00069	
0.00005									
3	A*	-42.158623							
0.00000		1	S	0.15206973	3	1	0.01781	0.00000	
			X	0.03868474	3	2	-0.03735	0.00000	
0.00000			Y	0.02957997	3	3	0.91579	0.00000	
1.00000			Z	0.00000082	3	4	-0.00001	0.00000	
0.00000		2	S	0.12722066	3	5	-0.49878	6.43682	-
0.36782			X	-0.04065531	3	6	0.01853	0.11962	-
0.00684			Y	-0.00284664	3	7	-0.62628	5.76708	-
0.32955			Z	-0.00000075	3	8	0.00005	-0.00010	
0.00001		3	S	-0.01033012	3	9	0.02804	1.17825	-
0.06733			X	-0.06886135	3	10	-0.03421	-0.85729	
0.04899			Y	0.02559967	3	11	0.00571	1.27282	-
0.07273			Z	-0.00000005	3	12	-0.00001	-0.00012	
0.00001		4	S	-0.15141506	3	13	0.00043	0.31866	-
0.01821			X	-0.11913775	3	14	0.00762	-0.41550	
0.02374			Y	0.07756469	3	15	-0.00359	0.15210	-
0.00869			Z	-0.00001261	3	16	-0.00001	-0.00004	
0.00000		5	S	0.08054210	3	17	-0.01059	-0.00671	
0.00038			X	-0.07371029	3	18	0.02682	0.00975	-
0.00056			Y	0.09631100	3	19	-0.00359	-0.23772	
0.01358			Z	-0.00000740	3	20	0.00000	0.00000	
0.00000		6	S	0.34693849	3	21	0.26281	-3.41571	
0.19518			X	0.00504137	3	22	-0.31567	3.49125	-
0.19950			Y	0.17425133	3	23	-0.09016	0.16747	-
0.00957			Z	-0.00000768	3	24	0.00000	0.00022	-
0.00001		7	S	-0.03842210	3	25	-0.03192	0.07719	-
0.00441			X	-0.05456021	3	26	0.00718	-0.03933	
0.00225			Y	-0.00344336	3	27	-0.03719	0.10670	-
0.00610			Z	0.00002126	3	28	-0.00003	0.00000	
0.00000		8	S	0.02829326	3	29	0.00024	0.00902	-
0.00029			X	-0.01102172	3	30	-0.00379	-0.00046	
0.00001			Y	0.01177334	3	31	0.00245	0.01168	-
0.00037			Z	-0.00000031	3	32	0.00003	0.00000	
0.00000		9	S	0.18501921	3	33	0.01276	1.00729	-
0.03223			X	0.03078756	3	34	0.03861	0.67013	-
0.02144			Y	-0.00104878	3	35	0.02024	0.94107	-
0.03011			Z	0.00001076	3	36	0.00000	0.00004	
0.00000		10	S	0.63911319	3	37	-0.01775	-0.95665	
0.03061			X	0.05612530	3	38	-0.00892	0.58022	-
0.01857			Y	-0.08370307	3	39	0.02661	0.93672	-
0.02997			Z	0.00002055	3	40	-0.00001	0.00000	
0.00000		11	S	-0.38791579	3	41	-0.00188	0.00454	-
0.00015									



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00017		X	0.04216118	3	42	0.00049	-0.00541	
0.00008		Y	-0.01704314	3	43	-0.00354	0.00234	-
0.00000		Z	0.00002932	3	44	0.00000	0.00000	
0.00025	12	S	-0.09494582	3	45	0.01047	0.00437	-
0.00021		X	-0.01264831	3	46	-0.01483	-0.00359	
0.00033		Y	-0.03446063	3	47	0.00935	0.00569	-
0.00000		Z	-0.00000629	3	48	0.00001	0.00000	
0.01167	13	S	0.07863470	3	49	-0.03524	0.17207	-
0.00915	14	S	0.26877481	3	50	0.02567	-0.13498	
0.23991	15	S	0.06557694	3	51	0.40225	-3.53874	
0.00192	16	S	0.03326268	3	52	0.01641	-0.02825	
0.00014	17	S	-0.12896059	3	53	-0.00121	0.00206	-
0.00038	18	S	-0.10495293	3	54	0.00132	0.00564	-
0.00009	19	S	-0.03428783	3	55	-0.00472	0.00127	-
0.00009	20	S	-0.03429761	3	56	-0.00471	0.00127	-
0.00000	4	A*	-39.643288	1	S	-0.13857086	0.00003	0.00000
0.00000		X	0.00998899	4	2	-0.00002	0.00000	
0.00000		Y	0.06854498	4	3	-0.00001	0.00000	
0.00000		Z	0.00000017	4	4	1.07722	0.00000	
1.00000	2	S	-0.26581419	4	5	-0.00001	-0.00008	
0.00000		X	0.12566414	4	6	-0.00006	0.00000	
0.00001		Y	0.01395737	4	7	0.00003	-0.00010	
0.11388		Z	0.00000872	4	8	0.65692	-1.99283	
0.00001	3	S	-0.00983201	4	9	0.00000	-0.00010	
0.00000		X	0.02467365	4	10	-0.00001	0.00007	
0.00001		Y	-0.12128074	4	11	0.00000	-0.00012	
0.01241		Z	0.00000719	4	12	-0.00015	-0.21709	
0.00000	4	S	-0.11693248	4	13	0.00001	-0.00005	
0.00000		X	-0.03254121	4	14	0.00003	0.00007	
0.00000		Y	-0.02436199	4	15	-0.00002	-0.00004	
0.00492		Z	-0.00000814	4	16	-0.31723	-0.08610	
0.00001	5	S	-0.08282707	4	17	-0.00001	-0.00010	
0.00001		X	0.00595920	4	18	0.00001	0.00014	-
0.00000		Y	0.04202199	4	19	0.00000	0.00000	
0.01359		Z	-0.00000280	4	20	-0.01429	-0.23776	
0.00002	6	S	-0.02152248	4	21	0.00004	-0.00034	
0.00002		X	0.01045015	4	22	-0.00007	0.00035	-
0.00001		Y	0.07978168	4	23	0.00001	0.00022	-
0.11466		Z	-0.00000155	4	24	0.65548	-2.00661	
0.00000	7	S	0.39569175	4	25	0.00000	0.00000	
0.00000		X	-0.12412594	4	26	-0.00001	0.00000	
0.00000		Y	-0.17223091	4	27	0.00001	0.00000	
0.00045		Z	0.00006473	4	28	-0.02329	-0.00787	
0.00000	8	S	0.50632197	4	29	0.00000	0.00000	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		X	0.15009680	4	30	0.00000	0.00000				
0.00000		Y	0.05435963	4	31	0.00000	0.00000				
0.00002		Z	-0.00007093	4	32	0.00275	-0.00056				
0.00000	9	S	-0.46035096	4	33	0.00001	0.00003				
0.00000		X	-0.06225392	4	34	0.00002	0.00002				
0.00000		Y	-0.02544880	4	35	-0.00002	0.00004				
0.00430		Z	-0.00001504	4	36	-0.11819	-0.13435				
0.00000	10	S	0.12341656	4	37	0.00001	0.00000				
0.00000		X	0.01311447	4	38	0.00002	0.00000				
0.00000		Y	-0.00422527	4	39	0.00000	0.00000				
0.00389		Z	0.00000403	4	40	-0.11345	-0.12154				
0.00000	11	S	-0.15817642	4	41	0.00000	0.00000				
0.00000		X	0.00661411	4	42	0.00000	0.00000				
0.00000		Y	-0.03937206	4	43	0.00000	0.00000				
0.00002		Z	-0.00000717	4	44	0.06776	-0.00059				
0.00000	12	S	0.20754166	4	45	0.00000	0.00000				
0.00000		X	-0.09621138	4	46	0.00000	0.00000				
0.00000		Y	0.00119538	4	47	0.00000	0.00000				
0.00002		Z	0.00005741	4	48	0.00122	-0.00036				
0.00000	13	S	-0.13284694	4	49	-0.00003	-0.00002				
0.00000	14	S	0.05344833	4	50	-0.00001	-0.00001				
0.00008	15	S	-0.05469256	4	51	-0.00013	0.00124	-			
0.00000	16	S	-0.02678897	4	52	0.00000	-0.00002				
0.00000	17	S	-0.06849117	4	53	0.00000	0.00000				
0.00000	18	S	0.04534505	4	54	-0.00001	0.00000				
0.00002	19	S	0.09422307	4	55	-0.00308	0.00022	-			
0.00001	20	S	0.09421410	4	56	0.00309	-0.00022				
0.34403	5	A*	-36.636635	1	S	0.31841293	5	1	0.31263	-6.02048	
0.00567		X	0.11778469	5	2	0.00407	0.09923	-			
0.36782		Y	-0.05833741	5	3	-0.49878	6.43682	-			
0.00000		Z	0.00000868	5	4	-0.00001	-0.00008				
1.00000	2	S	0.21652725	5	5	1.12481	0.00000				
0.00000		X	0.22120310	5	6	0.04789	0.00000				
0.00000		Y	0.13152948	5	7	0.02187	0.00000				
0.00000		Z	0.00001381	5	8	0.00000	0.00000				
0.33947	3	S	0.31771377	5	9	0.31486	-5.94080				
0.31703		X	0.00942549	5	10	-0.43897	5.54797	-			
0.17944		Y	0.12546992	5	11	0.25348	-3.14015				
0.00004		Z	-0.00000919	5	12	-0.00006	0.00069	-			
0.05445	4	S	0.22253557	5	13	-0.03421	-0.95289				
0.07329		X	-0.22867484	5	14	0.01831	1.28251	-			
0.00029		Y	0.10518257	5	15	0.01798	0.00508	-			
0.00001		Z	-0.00002624	5	16	0.00001	0.00011	-			
0.02690	5	S	0.29204169	5	17	-0.01570	-0.47077				

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.03235		X	-0.12346399	5	18	0.00158	0.56610	-			
		Y	-0.06636064	5	19	-0.00004	0.33287	-			
0.01902		Z	-0.00000493	5	20	0.00000	0.00003				
0.00000											
0.05351	6	S	0.23200566	5	21	-0.02731	-0.93642				
		X	-0.01294457	5	22	0.02026	0.62024	-			
0.03544		Y	-0.24465819	5	23	0.01017	1.09869	-			
0.06278		Z	0.00000428	5	24	-0.00001	0.00003				
0.00000											
0.05414	7	S	0.07206438	5	25	-0.00485	-0.94744				
		X	0.01652980	5	26	0.01025	0.64023	-			
0.03658		Y	0.06475684	5	27	-0.02518	-1.10332				
0.06305		Z	-0.00000511	5	28	-0.00004	0.00006				
0.00000											
0.00846	8	S	-0.03022936	5	29	-0.00446	-0.26426				
		X	0.02079988	5	30	-0.01735	0.02034	-			
0.00065		Y	-0.00037787	5	31	0.00694	-0.31942				
0.01022		Z	-0.00000013	5	32	0.00005	0.00008				
0.00000											
0.22125	9	S	-0.29808959	5	33	0.20264	-6.91415				
		X	0.00519453	5	34	0.42666	-5.79981				
0.18559		Y	0.04525793	5	35	0.21031	-3.01903				
0.09661		Z	-0.00001701	5	36	0.00003	-0.00041				
0.00001											
0.00069	10	S	-0.26485953	5	37	0.02165	-0.02161				
		X	-0.03210555	5	38	-0.00487	0.00884	-			
0.00028		Y	-0.03101921	5	39	-0.03979	0.02613	-			
0.00084		Z	-0.00000864	5	40	0.00001	0.00000				
0.00000											
0.00064	11	S	-0.29167810	5	41	0.01930	-0.02013				
		X	-0.03168632	5	42	-0.03718	0.02540	-			
0.00081		Y	-0.00102770	5	43	0.01810	-0.00414				
0.00013		Z	0.00000713	5	44	-0.00001	0.00000				
0.00000											
0.00314	12	S	0.00262795	5	45	0.02474	-0.05500				
		X	-0.02680583	5	46	-0.02497	0.05469	-			
0.00313		Y	0.00512948	5	47	0.02820	-0.06070				
0.00347		Z	0.00000936	5	48	0.00003	-0.00002				
0.00000											
0.11118	13	S	-0.13782603	5	49	-0.00079	-1.63994				
0.00069	14	S	-0.12246533	5	50	-0.01239	-0.01014				
0.09778	15	S	0.08174957	5	51	-0.01829	-1.44222				
0.00304	16	S	0.06188120	5	52	0.00916	-0.04490				
0.00052	17	S	-0.11414834	5	53	-0.01134	-0.00769				
0.00272	18	S	-0.03642746	5	54	0.01103	-0.04013				
0.00097	19	S	-0.00157934	5	55	-0.01050	-0.01430				
0.00097	20	S	-0.00158629	5	56	-0.01049	-0.01428				
0.00567	6	A*	-33.394650	1	S	-0.02601227	6	1	-0.01788	-0.09923	
0.11377		X	-0.03294796	6	2	0.07510	-1.99099				
		Y	-0.01867194	6	3	0.01853	0.11962	-			
0.00684		Z	-0.00000426	6	4	-0.00006	0.00000				
0.00000											
0.00000	2	S	0.06002469	6	5	0.04789	0.00000				

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

1.00000		X	-0.00742056	6	6	0.88341	0.00000	
0.00000		Y	-0.03396449	6	7	-0.05144	0.00000	
0.00000		Z	-0.00001097	6	8	0.00001	0.00000	
0.31703	3	S	0.18563916	6	9	0.39820	-5.54797	
0.22193		X	0.05929410	6	10	-0.42685	3.88370	-
0.18892		Y	-0.07641546	6	11	0.29256	-3.30611	
0.00004		Z	-0.00004858	6	12	-0.00011	0.00073	-
0.07329	4	S	-0.06040141	6	13	-0.02808	-1.28251	
0.09569		X	-0.12564579	6	14	-0.00629	1.67456	-
0.00042		Y	-0.14829512	6	15	0.02667	0.00743	-
0.00001		Z	-0.00004214	6	16	0.00001	0.00016	-
0.03235	5	S	-0.20987827	6	17	0.00160	-0.56610	
0.03681		X	-0.02086419	6	18	-0.01379	0.64415	-
0.02462		Y	0.02058531	6	19	-0.00886	0.43092	-
0.00000		Z	-0.00001166	6	20	0.00002	0.00004	
0.03544	6	S	-0.08383554	6	21	-0.00135	-0.62024	
0.01422		X	-0.04047168	6	22	-0.00638	0.24878	-
0.04519		Y	0.06651600	6	23	-0.01662	0.79082	-
0.00000		Z	-0.00000605	6	24	-0.00001	0.00002	
0.03658	7	S	0.14103337	6	25	-0.02011	-0.64023	
0.01542		X	0.35236287	6	26	0.00828	0.26983	-
0.04631		Y	0.11653330	6	27	-0.03851	-0.81036	
0.00000		Z	-0.00021381	6	28	-0.00006	0.00004	
0.00086	8	S	-0.41439533	6	29	-0.00816	-0.02689	
0.00122		X	0.00180723	6	30	-0.00123	-0.03798	
0.00111		Y	-0.03544350	6	31	0.00038	-0.03473	
0.00000		Z	-0.00000667	6	32	0.00006	0.00001	
0.26632	9	S	0.06115162	6	33	-0.35222	8.32265	-
0.19019		X	0.01525837	6	34	-0.56849	5.94337	-
0.13142		Y	0.03393385	6	35	-0.30553	4.10694	-
0.00002		Z	-0.00001118	6	36	-0.00007	0.00056	-
0.00037	10	S	0.08533245	6	37	0.00288	-0.01144	
0.00008		X	-0.00012657	6	38	0.00123	0.00242	-
0.00047		Y	0.02073320	6	39	-0.00432	0.01455	-
0.00000		Z	0.00000102	6	40	0.00000	0.00000	
0.00105	11	S	-0.17281365	6	41	0.02061	-0.03285	
0.00132		X	-0.06211982	6	42	-0.03075	0.04122	-
0.00023		Y	-0.15827379	6	43	0.01638	-0.00710	
0.00000		Z	-0.00008499	6	44	0.00000	0.00000	
0.00313	12	S	0.49450523	6	45	0.02320	-0.05469	
0.00283		X	0.01645367	6	46	-0.02088	0.04958	-
0.00364		Y	0.06092036	6	47	0.02240	-0.06376	
0.00000		Z	-0.00000851	6	48	0.00002	-0.00002	
0.07606	13	S	-0.03171285	6	49	0.02142	1.12189	-
0.00046	14	S	0.03322048	6	50	0.00103	-0.00682	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.04943		15	S	-0.00117546	6	51	-0.00252	0.72915	-
0.00360		16	S	-0.10915075	6	52	0.00377	-0.05306	
0.00073		17	S	-0.14729172	6	53	-0.01122	-0.01075	
0.00314		18	S	0.26701003	6	54	0.01018	-0.04638	
0.00081		19	S	0.21457398	6	55	-0.01044	-0.01191	
0.00081		20	S	0.21456866	6	56	-0.01042	-0.01190	
0.36782	7 A* -30.603544	1	S	0.49563634	7	1	0.48646	-6.43682	
0.00684			X	-0.02675248	7	2	0.00603	0.11962	-
0.32955			Y	0.04728834	7	3	-0.62628	5.76708	-
0.00001			Z	-0.00001231	7	4	0.00003	-0.00010	
0.00000		2	S	0.08293352	7	5	0.02187	0.00000	
0.00000			X	-0.12384313	7	6	-0.05144	0.00000	
1.00000			Y	0.24454935	7	7	0.95930	0.00000	
0.00000			Z	-0.00002348	7	8	-0.00004	0.00000	
0.17944		3	S	-0.35616216	7	9	-0.26752	3.14015	-
0.18892			X	-0.06135741	7	10	0.32713	-3.30611	
0.00493			Y	0.01911293	7	11	-0.11448	-0.08623	
0.00002			Z	-0.00001015	7	12	0.00005	-0.00041	
0.00029		4	S	-0.28469095	7	13	0.01794	-0.00508	
0.00042			X	0.12403354	7	14	-0.02144	0.00743	-
0.01153			Y	-0.00303831	7	15	-0.01402	-0.20173	
0.00000			Z	0.00000227	7	16	0.00000	0.00000	
0.01902		5	S	-0.15189031	7	17	-0.00073	-0.33287	
0.02462			X	-0.06440917	7	18	-0.00733	0.43092	-
0.00941			Y	0.07932866	7	19	-0.00426	0.16470	-
0.00000			Z	-0.00001229	7	20	-0.00001	0.00002	
0.06278		6	S	0.21033031	7	21	-0.03014	-1.09869	
0.04519			X	-0.20919318	7	22	0.02809	0.79082	-
0.06875			Y	-0.06773020	7	23	-0.00422	1.20320	-
0.00000			Z	-0.00001891	7	24	0.00000	0.00004	
0.06305		7	S	-0.06886183	7	25	0.01575	1.10332	-
0.04631			X	0.02454004	7	26	0.01305	-0.81036	
0.06835			Y	-0.21171071	7	27	0.01513	1.19611	-
0.00000			Z	-0.00002737	7	28	0.00006	-0.00008	
0.01351		8	S	0.07849561	7	29	-0.00036	0.42219	-
0.00111			X	0.04334650	7	30	0.00830	-0.03473	
0.01616			Y	-0.05492362	7	31	-0.01563	0.50513	-
0.00000			Z	-0.00001960	7	32	-0.00004	-0.00013	
0.13863		9	S	-0.02335529	7	33	-0.18564	4.33227	-
0.13142			X	0.00044450	7	34	-0.34611	4.10694	-
0.00613			Y	0.10688195	7	35	-0.10367	0.19141	-
0.00001			Z	-0.00001654	7	36	-0.00002	0.00029	-
0.00108		10	S	-0.10200754	7	37	0.02554	-0.03382	
0.00047			X	-0.09224325	7	38	-0.00413	0.01455	-

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00130			Y	-0.09548500	7	39	-0.03891	0.04048	-	
0.00000			Z	-0.00001282	7	40	0.00000	0.00000		
0.00017			11	S	0.16313104	7	41	-0.00876	0.00536	-
0.00023			X	0.10394759	7	42	0.01533	-0.00710		
0.00004			Y	-0.05406934	7	43	-0.00591	-0.00116		
0.00000			Z	-0.00001973	7	44	0.00000	0.00000		
0.00347			12	S	0.18342918	7	45	-0.02068	0.06070	-
0.00364			X	0.02359156	7	46	0.01858	-0.06376		
0.00359			Y	-0.05532111	7	47	-0.01593	0.06288	-	
0.00000			Z	-0.00001603	7	48	-0.00002	0.00002		
0.11265			13	S	-0.07736526	7	49	-0.00268	1.66151	-
0.00084			14	S	-0.11569158	7	50	-0.01505	-0.01238	
0.11000			15	S	0.26821187	7	51	-0.04357	-1.62247	
0.00212			16	S	-0.08404127	7	52	0.00369	-0.03121	
0.00001			17	S	0.08190670	7	53	0.00765	-0.00019	
0.00202			18	S	0.09062400	7	54	-0.00610	0.02974	-
0.00105			19	S	0.10892774	7	55	0.00703	0.01543	-
0.00105			20	S	0.10892545	7	56	0.00701	0.01542	-
8	A*	-29.806129	1	S	-0.16505045	8	1	0.00001	0.00008	
0.00000			X	0.06409643	8	2	-0.00007	0.00000		
0.00000			Y	0.06996559	8	3	0.00005	-0.00010		
0.11388			Z	0.00000523	8	4	0.65692	-1.99283		
0.00000			2	S	-0.26175162	8	5	0.00000	0.00000	
0.00000			X	-0.13425313	8	6	0.00001	0.00000		
0.00000			Y	-0.01727238	8	7	-0.00004	0.00000		
1.00000			Z	-0.00001451	8	8	0.85870	0.00000		
0.00004			3	S	-0.30912635	8	9	0.00007	-0.00069	
0.00004			X	0.09107893	8	10	-0.00012	0.00073	-	
0.00002			Y	0.01475315	8	11	0.00006	-0.00041		
0.11186			Z	-0.00000904	8	12	0.60625	-1.95749		
0.00001			4	S	0.05954248	8	13	-0.00002	-0.00011	
0.00001			X	0.04288372	8	14	0.00002	0.00016	-	
0.00000			Y	0.23322766	8	15	0.00001	0.00000		
0.01153			Z	-0.00002079	8	16	-0.04140	-0.20176		
0.00000			5	S	0.48153940	8	17	0.00002	-0.00003	
0.00000			X	0.01569606	8	18	0.00003	0.00004		
0.00000			Y	0.05175919	8	19	-0.00001	0.00002		
0.00507			Z	0.00000551	8	20	-0.30391	-0.08869		
0.00000			6	S	0.17290555	8	21	-0.00001	-0.00003	
0.00000			X	0.20957260	8	22	-0.00001	0.00002		
0.00000			Y	-0.09665556	8	23	0.00001	0.00004		
0.01129			Z	0.00001841	8	24	0.07702	-0.19766		
0.00000			7	S	-0.05216517	8	25	0.00000	-0.00006	
0.00000			X	0.11722799	8	26	0.00009	0.00004		

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		Y	-0.18126737	8	27	-0.00004	-0.00008	
		Z	-0.00008555	8	28	0.10467	-0.20040	
0.01145				8	S	-0.01717108	-0.00001	-0.00010
0.00000		X	0.01035539	8	30	-0.00010	0.00001	
0.00000		Y	-0.05331346	8	31	0.00000	-0.00013	
0.00000		Z	-0.00002225	8	32	-0.13578	-0.04019	
0.00129				9	S	0.21369013	-0.00004	0.00059
0.00002		X	-0.08393880	8	34	-0.00007	0.00056	-
0.00002		Y	-0.06684747	8	35	0.00003	0.00029	-
0.00001		Z	0.00000878	8	36	0.22213	-1.94641	
0.06229				10	S	-0.15704395	0.00000	0.00000
0.00000		X	0.04402011	8	38	0.00001	0.00000	
0.00000		Y	-0.06488095	8	39	0.00000	0.00000	
0.00000		Z	0.00000325	8	40	-0.02900	-0.00250	
0.00008				11	S	-0.15386301	0.00000	0.00000
0.00000		X	-0.02058947	8	42	-0.00001	0.00000	
0.00000		Y	0.02189410	8	43	0.00001	0.00000	
0.00000		Z	-0.00003946	8	44	0.00232	-0.00231	
0.00007				12	S	0.28074995	0.00003	0.00002
0.00000		X	0.00401207	8	46	-0.00004	-0.00002	
0.00000		Y	-0.06745174	8	47	0.00004	0.00002	
0.00000		Z	-0.00001894	8	48	-0.02174	-0.00788	
0.00045				13	S	0.10085919	0.00004	-0.00039
0.00003				14	S	-0.03823706	0.00000	0.00000
0.00000				15	S	-0.09283305	-0.00001	0.00016
0.00001				16	S	0.25885412	-0.00002	0.00000
0.00000				17	S	-0.04507174	0.00000	0.00000
0.00000				18	S	0.08010916	0.00002	0.00002
0.00000				19	S	0.15950549	0.02105	0.00381
0.00026				20	S	0.15948728	-0.02109	-0.00380
0.00026								
9	A*		-25.443235	1	S	0.02007428	-0.01125	-1.01384
0.05793		X	0.14326201	9	2	-0.00431	-0.67796	
0.03874		Y	0.30505669	9	3	0.02804	1.17825	-
0.06733		Z	0.00000411	9	4	0.00000	-0.00010	
0.00001				2	S	-0.35214540	0.31486	-5.94080
0.33947		X	0.06259578	9	6	0.39820	-5.54797	
0.31703		Y	-0.09183031	9	7	-0.26752	3.14015	-
0.17944		Z	0.00001810	9	8	0.00007	-0.00069	
0.00004				3	S	0.09109128	1.08078	0.00000
1.00000		X	0.13089262	9	10	-0.00771	0.00000	
0.00000		Y	-0.14563417	9	11	-0.00604	0.00000	
0.00000		Z	0.00001783	9	12	0.00004	0.00000	
0.00000				4	S	0.00283065	0.32249	-5.94709
0.33983		X	-0.03326489	9	14	-0.38592	5.52627	-
0.31579								

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.18218		Y	-0.16288544	9	15	-0.27717	3.18811	-			
		Z	0.00000165	9	16	0.00000	0.00025	-			
0.00001											
0.05868	5	S	-0.11132203	9	17	-0.01342	-1.02686				
		X	-0.14009880	9	18	0.00081	0.66957	-			
0.03826											
0.06867		Y	0.06797380	9	19	0.02918	1.20180	-			
		Z	-0.00001896	9	20	0.00000	-0.00001				
0.00000											
0.02420	6	S	0.35666633	9	21	-0.01473	-0.42341				
		X	-0.14019208	9	22	0.00166	-0.00409				
0.00023											
0.03390		Y	0.05585619	9	23	0.00002	0.59326	-			
		Z	-0.00002187	9	24	-0.00001	-0.00002				
0.00000											
0.33216	7	S	0.07665341	9	25	0.29422	-5.81281				
		X	0.00856714	9	26	-0.03514	0.01266	-			
0.00072											
0.35846		Y	0.16658978	9	27	0.47354	-6.27313				
		Z	0.00002031	9	28	0.00005	-0.00017				
0.00001											
0.02701	8	S	-0.03165798	9	29	0.01060	-0.84405				
		X	-0.07744494	9	30	0.01252	-0.42985				
0.01376											
0.02809		Y	0.06782827	9	31	-0.08240	-0.87789				
		Z	0.00002777	9	32	-0.00002	0.00021	-			
0.00001											
0.02074	9	S	0.10909752	9	33	0.00613	-0.64808				
		X	-0.15395284	9	34	-0.05657	-0.75963				
0.02431											
0.00038		Y	-0.26504496	9	35	0.01122	0.01185	-			
		Z	0.00005012	9	36	-0.00001	-0.00007				
0.00000											
0.00017	10	S	-0.11457585	9	37	-0.00005	-0.00519				
		X	-0.19265968	9	38	-0.00243	-0.00004				
0.00000											
0.00022		Y	-0.31385982	9	39	-0.00036	0.00674	-			
		Z	-0.00003205	9	40	0.00000	0.00000				
0.00000											
0.01989	11	S	0.02824783	9	41	-0.01037	-0.62154				
		X	-0.08114599	9	42	0.03381	0.72948	-			
0.02334											
0.00080		Y	-0.08991645	9	43	-0.00321	0.02514	-			
		Z	-0.00001387	9	44	0.00000	0.00008				
0.00000											
0.05698	12	S	-0.11722363	9	45	-0.01833	-0.99709				
		X	0.00424143	9	46	0.01631	0.69745	-			
0.03985											
0.06527		Y	0.11869641	9	47	-0.02943	-1.14220				
		Z	0.00002476	9	48	-0.00002	-0.00050				
0.00003											
0.04084	13	S	0.20925716	9	49	-0.01632	-0.60242				
0.00041	14	S	-0.24325590	9	50	0.00108	-0.00599				
0.00831	15	S	0.02685764	9	51	0.04290	-0.12263				
0.00842	16	S	-0.12001833	9	52	0.04183	-0.12413				
0.00644	17	S	-0.07346748	9	53	0.03311	-0.09506				
0.05039	18	S	0.02571332	9	54	-0.01820	-0.74321				
0.01352	19	S	-0.10339360	9	55	0.02907	-0.19942				
0.01352	20	S	-0.10336517	9	56	0.02906	-0.19942				
	10	A*	-24.583761	1	S	-0.15531603	10	1	0.02177	0.67796	-
0.03874											
		X	0.11846443	10	2	0.00077	0.27619	-			
0.01578											



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.04899		Y	-0.04618853	10	3	-0.03421	-0.85729	
0.00000		Z	0.00001592	10	4	-0.00001	0.00007	
0.31703	2	S	0.15227491	10	5	-0.43897	5.54797	-
0.22193		X	0.10641994	10	6	-0.42685	3.88370	-
0.18892		Y	-0.16145802	10	7	0.32713	-3.30611	
0.00004		Z	0.00001276	10	8	-0.00012	0.00073	-
0.00000	3	S	0.11574120	10	9	-0.00771	0.00000	
1.00000		X	-0.27873659	10	10	0.88226	0.00000	
0.00000		Y	-0.11951105	10	11	-0.00644	0.00000	
0.00000		Z	-0.00003524	10	12	-0.00001	0.00000	
0.31579	4	S	-0.43300307	10	13	0.44897	-5.52627	
0.21882		X	-0.05299396	10	14	-0.41141	3.82927	-
0.19086		Y	0.05361179	10	15	-0.33818	3.33999	-
0.00001		Z	-0.00001773	10	16	-0.00008	0.00026	-
0.03826	5	S	0.10409912	10	17	-0.02293	-0.66957	
0.01456		X	-0.06046404	10	18	-0.00126	0.25476	-
0.04873		Y	0.26944378	10	19	0.03342	0.85283	-
0.00000		Z	-0.00001200	10	20	0.00001	-0.00001	
0.00023	6	S	0.17909715	10	21	0.00175	0.00409	-
0.00448		X	0.17488313	10	22	0.00124	-0.07845	
0.00035		Y	-0.01613540	10	23	-0.00089	-0.00616	
0.00000		Z	0.00001282	10	24	0.00003	0.00000	
0.00072	7	S	0.11655363	10	25	0.00138	-0.01266	
0.10864		X	-0.01139418	10	26	0.06551	-1.90115	
0.00088		Y	0.13187286	10	27	-0.00135	-0.01539	
0.00000		Z	-0.00004191	10	28	0.00005	0.00000	
0.01849	8	S	-0.15440100	10	29	0.00386	0.57770	-
0.00534		X	0.03300757	10	30	0.00115	0.16674	-
0.02081		Y	0.08922822	10	31	-0.01048	0.65032	-
0.00001		Z	-0.00003247	10	32	-0.00004	-0.00016	
0.03252	9	S	-0.09959665	10	33	0.00627	1.01640	-
0.03755		X	0.12201662	10	34	0.05414	1.17332	-
0.00064		Y	-0.01261014	10	35	0.00782	-0.02004	
0.00000		Z	0.00000191	10	36	0.00002	0.00013	
0.00000	10	S	-0.12124715	10	37	0.00047	0.00005	
0.00002		X	0.06688458	10	38	-0.00491	-0.00053	
0.00000		Y	-0.13428979	10	39	0.00119	-0.00007	
0.00000		Z	0.00000716	10	40	-0.00001	0.00000	
0.03121	11	S	0.16996911	10	41	-0.02735	-0.97542	
0.03609		X	0.42759106	10	42	0.04010	1.12778	-
0.00136		Y	-0.06052015	10	43	-0.02615	0.04254	-
0.00000		Z	0.00003579	10	44	0.00002	0.00013	
0.03985	12	S	0.01243943	10	45	-0.00608	-0.69745	
0.01816		X	-0.00149149	10	46	-0.00823	0.31782	-
0.04966		Y	0.00571643	10	47	0.01719	-0.86908	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00002		Z	-0.00002321	10	48	0.00000	-0.00038			
0.04868		13	S	-0.02412890	10	49	0.00026	0.71810	-	
0.00011		14	S	-0.03005845	10	50	-0.00190	-0.00166		
0.00702		15	S	-0.16267611	10	51	-0.03823	0.10348	-	
0.00698		16	S	0.11516177	10	52	0.03655	-0.10289		
0.00851		17	S	0.25974256	10	53	0.04258	-0.12549		
0.05309		18	S	0.01121490	10	54	0.00846	-0.78306		
0.00791		19	S	0.00304243	10	55	0.00416	-0.11664		
0.00791		20	S	0.00301705	10	56	0.00414	-0.11674		
0.06733	11 A*	-23.019392	1	S	-0.08099990	11	1	-0.01426	-1.17825	
0.04899			X	0.20713916	11	2	0.02087	-0.85729		
0.07273			Y	-0.08346763	11	3	0.00571	1.27282	-	
0.00001			Z	0.00003373	11	4	0.00000	-0.00012		
0.17944			2	S	0.02787019	11	5	0.25348	-3.14015	
0.18892			X	0.25747424	11	6	0.29256	-3.30611		
0.00493			Y	0.01026824	11	7	-0.11448	-0.08623		
0.00002			Z	0.00004808	11	8	0.00006	-0.00041		
0.00000			3	S	0.01963225	11	9	-0.00604	0.00000	
0.00000			X	-0.05042241	11	10	-0.00644	0.00000		
1.00000			Y	0.31541145	11	11	0.89232	0.00000		
0.00000			Z	-0.00000396	11	12	0.00001	0.00000		
0.18218			4	S	-0.00853873	11	13	0.25262	-3.18811	
0.19086			X	-0.17668776	11	14	-0.28367	3.33999	-	
0.00191			Y	0.00179113	11	15	-0.11873	-0.03342		
0.00001			Z	-0.00004303	11	16	0.00000	0.00015	-	
0.06867			5	S	-0.11859430	11	17	-0.01196	-1.20180	
0.04873			X	-0.20203713	11	18	-0.02344	0.85283	-	
0.07488			Y	-0.07494209	11	19	0.00140	1.31033	-	
0.00000			Z	-0.00002436	11	20	0.00000	-0.00001		
0.03390			6	S	0.01482356	11	21	-0.00005	-0.59326	
0.00035			X	-0.00629192	11	22	0.00062	-0.00616		
0.04659			Y	-0.12095781	11	23	-0.01587	0.81526	-	
0.00000			Z	0.00000720	11	24	-0.00001	-0.00003		
0.35846			7	S	-0.35501459	11	25	-0.49272	6.27313	-
0.00088			X	-0.07350630	11	26	0.03462	-0.01539		
0.32738			Y	-0.10431167	11	27	-0.63942	5.72907	-	
0.00001			Z	0.00001606	11	28	-0.00006	0.00021	-	
0.03775			8	S	0.22129934	11	29	-0.00836	1.17984	-
0.02081			X	-0.19921091	11	30	0.01030	0.65032	-	
0.03765			Y	-0.08844205	11	31	0.06917	1.17647	-	
0.00001			Z	0.00007182	11	32	0.00002	-0.00032		
0.00051			9	S	-0.01586268	11	33	0.00452	-0.01585	
0.00064			X	-0.08354621	11	34	-0.03482	-0.02004		
0.00357			Y	-0.28654280	11	35	0.00204	-0.11145		

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		Z	0.00008591	11	36	-0.00001	0.00000	
0.00028		10	S	0.04622369	11	37	0.00146	-0.00866
0.00000		X	0.05046391	11	38	-0.00175	-0.00007	
0.00036		Y	0.12597558	11	39	-0.00072	0.01122	-
0.00000		Z	0.00001066	11	40	0.00000	0.00000	
0.00108		11	S	0.09300070	11	41	-0.00483	-0.03362
0.00136		X	0.11570985	11	42	0.02170	0.04254	-
0.00336		Y	-0.20477498	11	43	-0.00787	-0.10504	
0.00000		Z	-0.00009039	11	44	0.00000	0.00000	
0.06527		12	S	0.10864817	11	45	0.01760	1.14220
0.04966		X	0.22974917	11	46	-0.04180	-0.86908	
0.06917		Y	-0.11084145	11	47	0.00645	1.21042	-
0.00004		Z	-0.00015902	11	48	0.00003	0.00063	-
0.02009		13	S	0.20693648	11	49	-0.00816	0.29634
0.00056		14	S	0.07566691	11	50	0.00174	-0.00822
0.00874		15	S	-0.19195288	11	51	0.02922	-0.12896
0.00895		16	S	-0.20546509	11	52	0.02769	-0.13195
0.00196		17	S	0.00136387	11	53	0.02041	-0.02897
0.03647		18	S	0.15678075	11	54	-0.00021	0.53794
0.01548		19	S	0.11306305	11	55	-0.02816	0.22829
0.01548		20	S	0.11305474	11	56	-0.02816	0.22829
0.00001	12 A*							
0.00000	-21.753393	1	S	-0.06698944	12	1	0.00000	0.00010
0.00001		X	-0.02088853	12	2	0.00000	0.00007	
0.00001		Y	-0.10525004	12	3	-0.00001	-0.00012	
0.01241		Z	0.00000025	12	4	-0.00015	-0.21709	
0.00004		2	S	0.13088286	12	5	-0.00006	0.00069
0.00004		X	-0.13224250	12	6	-0.00011	0.00073	-
0.00002		Y	-0.00634560	12	7	0.00005	-0.00041	
0.11186		Z	-0.00002092	12	8	0.60625	-1.95749	
0.00000		3	S	-0.05759262	12	9	0.00004	0.00000
0.00000		X	-0.00681530	12	10	-0.00001	0.00000	
0.00000		Y	-0.02654200	12	11	0.00001	0.00000	
1.00000		Z	-0.00000002	12	12	1.16145	0.00000	
0.00001		4	S	-0.06367748	12	13	-0.00001	-0.00025
0.00001		X	0.10122703	12	14	-0.00007	0.00026	-
0.00001		Y	-0.19354814	12	15	0.00002	0.00015	-
0.11202		Z	-0.00002816	12	16	0.60934	-1.96027	
0.00000		5	S	0.06077419	12	17	0.00001	0.00001
0.00000		X	-0.05066430	12	18	0.00000	-0.00001	
0.00000		Y	0.24247910	12	19	0.00000	-0.00001	
0.01259		Z	-0.00002028	12	20	-0.05826	-0.22039	
0.00000		6	S	0.09978361	12	21	-0.00001	0.00002
0.00000		X	0.19808652	12	22	0.00001	0.00000	
0.00000		Y	0.01962234	12	23	-0.00001	-0.00003	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00449		Z	0.00001283	12	24	-0.29986	-0.07849	
0.00001		7 S	-0.11049160	12	25	0.00000	0.00017	-
0.00000		X	-0.09367590	12	26	0.00014	0.00000	
0.00001		Y	0.04928462	12	27	-0.00002	0.00021	-
0.10864		Z	0.00009957	12	28	0.32401	-1.90118	
0.00001		8 S	0.16227676	12	29	0.00000	-0.00029	
0.00001		X	-0.08625784	12	30	-0.00004	-0.00016	
0.00001		Y	-0.03145465	12	31	0.00002	-0.00032	
0.00485		Z	0.00009082	12	32	-0.08046	-0.15168	
0.00000		9 S	-0.06385988	12	33	0.00001	0.00010	
0.00000		X	0.15057921	12	34	0.00003	0.00013	
0.00000		Y	0.20499566	12	35	-0.00002	0.00000	
0.00358		Z	-0.00003877	12	36	-0.11480	-0.11176	
0.00000		10 S	-0.11587405	12	37	0.00000	0.00000	
0.00000		X	0.15866326	12	38	-0.00001	0.00000	
0.00000		Y	-0.12092948	12	39	0.00000	0.00000	
0.00002		Z	0.00002398	12	40	0.06808	-0.00053	
0.00000		11 S	0.07437544	12	41	0.00000	-0.00010	
0.00000		X	-0.35970247	12	42	0.00000	0.00013	
0.00000		Y	-0.39934006	12	43	-0.00001	0.00000	
0.00341		Z	-0.00022362	12	44	-0.10483	-0.10651	
0.00003		12 S	-0.08515460	12	45	-0.00001	0.00050	-
0.00002		X	0.19855754	12	46	0.00001	-0.00038	
0.00004		Y	0.17073403	12	47	-0.00004	0.00063	-
0.01216		Z	-0.00004170	12	48	-0.01256	-0.21286	
0.00000		13 S	-0.12921751	12	49	-0.00001	-0.00007	
0.00000		14 S	0.03546300	12	50	0.00001	0.00000	
0.00000		15 S	-0.05994965	12	51	0.00000	0.00002	
0.00000		16 S	0.07943039	12	52	0.00000	-0.00001	
0.00000		17 S	-0.34489197	12	53	0.00001	-0.00001	
0.00004		18 S	0.24663191	12	54	-0.00001	0.00056	-
0.00482		19 S	-0.10213874	12	55	0.02622	0.07115	-
0.00481		20 S	-0.10203935	12	56	-0.02622	-0.07099	
0.02622	13 A*	-21.275778	1 S	-0.21534440	13	1	-0.01476	-0.45881
0.03176		X	0.05847305	13	2	-0.00006	-0.55587	
0.01821		Y	-0.03068827	13	3	0.00043	0.31866	-
0.00000		Z	0.00000373	13	4	0.00001	-0.00005	
0.05445		2 S	0.20347430	13	5	-0.03421	-0.95289	
0.07329		X	-0.02189033	13	6	-0.02808	-1.28251	
0.00029		Y	-0.18799837	13	7	0.01794	-0.00508	
0.00001		Z	-0.00000510	13	8	-0.00002	-0.00011	
0.33983		3 S	0.01583746	13	9	0.32249	-5.94709	
0.31579		X	-0.11341723	13	10	0.44897	-5.52627	
0.18218		Y	0.16678920	13	11	0.25262	-3.18811	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00001		Z	-0.00000373	13	12	-0.00001	-0.00025	
1.00000	4	S	0.12227317	13	13	1.11933	0.00000	
0.00000		X	0.06250079	13	14	-0.07319	0.00000	
0.00000		Y	0.03978397	13	15	0.02502	0.00000	
0.00000		Z	0.00002334	13	16	-0.00003	0.00000	
0.34311	5	S	-0.05818161	13	17	0.31042	-6.00443	
0.01240		X	0.05355831	13	18	0.00814	-0.21694	
0.36693		Y	-0.11454361	13	19	-0.49649	6.42136	-
0.00002		Z	0.00000503	13	20	0.00001	-0.00032	
0.05266	6	S	0.07827578	13	21	-0.02796	-0.92162	
0.03575		X	-0.05023403	13	22	-0.02366	-0.62554	
0.06137		Y	0.31264630	13	23	0.01227	1.07401	-
0.00000		Z	-0.00003550	13	24	0.00002	-0.00008	
0.05388	7	S	-0.15352039	13	25	-0.01371	-0.94295	
0.03603		X	-0.05257387	13	26	-0.00470	-0.63048	
0.06299		Y	-0.10209505	13	27	-0.01934	-1.10237	
0.00000		Z	-0.00000004	13	28	0.00002	-0.00005	
0.00097	8	S	0.05234389	13	29	0.01079	-0.03016	
0.00076		X	0.01603013	13	30	0.01355	-0.02390	
0.00096		Y	-0.07167315	13	31	0.03932	-0.02995	
0.00000		Z	-0.00000794	13	32	-0.00003	0.00000	
0.00067	9	S	-0.06630524	13	33	0.01431	-0.02083	
0.00084		X	0.21811333	13	34	0.04979	-0.02619	
0.00015		Y	0.16304749	13	35	0.00791	-0.00470	
0.00000		Z	-0.00004586	13	36	0.00001	0.00000	
0.00068	10	S	0.06419341	13	37	0.01563	-0.02135	
0.00029		X	-0.37885508	13	38	0.01936	-0.00903	
0.00082		Y	-0.39320314	13	39	-0.04281	0.02572	-
0.00000		Z	-0.00009438	13	40	0.00000	0.00000	
0.22014	11	S	-0.05055230	13	41	0.21233	-6.87946	
0.18771		X	-0.09332940	13	42	-0.40171	5.86584	-
0.09050		Y	0.14397703	13	43	0.22050	-2.82824	
0.00003		Z	0.00003584	13	44	-0.00007	0.00096	-
0.02749	12	S	0.08143519	13	45	-0.00831	-0.48112	
0.00060		X	0.04581356	13	46	0.00212	0.01046	-
0.03831		Y	-0.17683089	13	47	0.00202	-0.67044	
0.00001		Z	-0.00007482	13	48	0.00000	-0.00023	
0.00217	13	S	-0.12420341	13	49	0.00561	-0.03200	
0.00236	14	S	-0.33879536	13	50	0.00427	-0.03474	
0.00297	15	S	-0.15416873	13	51	0.00672	-0.04375	
0.09781	16	S	-0.04609300	13	52	-0.01577	-1.44273	
0.08847	17	S	-0.00838870	13	53	-0.01591	-1.30498	
0.07476	18	S	-0.05099605	13	54	0.00895	-1.10278	
0.00622	19	S	0.11924099	13	55	0.00268	-0.09175	
0.00623	20	S	0.11918996	13	56	0.00267	-0.09183	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

14	A*	-20.097111	1	S	0.14553469	14	1	-0.00081	0.55587	-
0.03176				X	-0.19349991	14	2	-0.01359	0.63870	-
0.03650				Y	0.10211512	14	3	0.00762	-0.41550	
0.02374				Z	-0.00002051	14	4	0.00003	0.00007	
0.00000			2	S	0.04145174	14	5	0.01831	1.28251	-
0.07329				X	0.15030499	14	6	-0.00629	1.67456	-
0.09569				Y	-0.06460538	14	7	-0.02144	0.00743	-
0.00042				Z	0.00005100	14	8	0.00002	0.00016	-
0.00001			3	S	0.03905622	14	9	-0.38592	5.52627	-
0.31579				X	-0.22351401	14	10	-0.41141	3.82927	-
0.21882				Y	-0.10046841	14	11	-0.28367	3.33999	-
0.19086				Z	-0.00002908	14	12	-0.00007	0.00026	-
0.00001			4	S	-0.07853340	14	13	-0.07319	0.00000	
0.00000				X	0.17674761	14	14	0.85459	0.00000	
1.00000				Y	0.08142831	14	15	0.06764	0.00000	
0.00000				Z	-0.00003599	14	16	0.00001	0.00000	
0.00000			5	S	0.11797481	14	17	0.01015	0.21694	-
0.01240				X	0.34113586	14	18	0.07609	-1.97686	
0.11296				Y	0.04096202	14	19	-0.00674	-0.26160	
0.01495				Z	0.00002115	14	20	-0.00007	0.00001	
0.00000			6	S	-0.16147478	14	21	-0.00027	0.62554	-
0.03575				X	-0.10060300	14	22	-0.00675	0.26730	-
0.01527				Y	0.08040295	14	23	0.01726	-0.79199	
0.04526				Z	-0.00001350	14	24	-0.00002	0.00006	
0.00000			7	S	-0.09368312	14	25	0.02520	0.63048	-
0.03603				X	-0.07986526	14	26	-0.00012	0.25888	-
0.01479				Y	0.18596964	14	27	0.03518	0.80108	-
0.04578				Z	-0.00004090	14	28	-0.00004	0.00003	
0.00000			8	S	0.02545747	14	29	-0.00992	0.03099	-
0.00099				X	-0.22584081	14	30	-0.01130	0.02224	-
0.00071				Y	0.12551965	14	31	-0.03355	0.03239	-
0.00104				Z	0.00004407	14	32	0.00004	-0.00001	
0.00000			9	S	-0.20282036	14	33	-0.01422	0.03389	-
0.00108				X	0.14719416	14	34	-0.03485	0.04236	-
0.00136				Y	-0.36529019	14	35	-0.00614	0.00803	-
0.00026				Z	0.00018562	14	36	-0.00001	0.00000	
0.00000			10	S	0.03302893	14	37	-0.00313	0.01168	-
0.00037				X	-0.10344544	14	38	0.00139	0.00272	-
0.00009				Y	0.03395583	14	39	0.00338	-0.01479	
0.00047				Z	-0.00001937	14	40	0.00000	0.00000	
0.00000			11	S	-0.06253999	14	41	0.37052	-8.41502	
0.26928				X	-0.12004383	14	42	-0.54710	6.17399	-
0.19757				Y	0.01288618	14	43	0.34668	-3.90919	
0.12509				Z	-0.00020227	14	44	-0.00013	0.00132	-
0.00004										

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00060		12	S	0.07827742	14	45	0.00905	-0.01046		
			X	0.20566233	14	46	0.00334	-0.09070		
0.00518			Y	-0.04978865	14	47	0.00494	-0.01570		
0.00090			Z	-0.00023067	14	48	0.00001	-0.00001		
0.00000		13	S	0.23468901	14	49	-0.00464	0.03990	-	
0.00270		14	S	-0.03927515	14	50	-0.00014	0.00360	-	
0.00024		15	S	0.23185709	14	51	-0.00313	0.05208	-	
0.00353		16	S	0.29631755	14	52	0.00413	-0.70091		
0.04752		17	S	-0.06966027	14	53	-0.03518	-1.61894		
0.10976		18	S	0.11196883	14	54	0.00310	-0.48830		
0.03310		19	S	0.07397232	14	55	-0.00102	-0.00484		
0.00033		20	S	0.07385524	14	56	-0.00101	-0.00489		
0.00033										
0.01821	15 A*	-19.041492	1	S	-0.00716875	15	1	0.00004	-0.31866	
			X	-0.23464182	15	2	0.00794	-0.41550		
0.02374			Y	0.03395433	15	3	-0.00359	0.15210	-	
0.00869			Z	-0.00005673	15	4	-0.00002	-0.00004		
0.00000										
0.00029			2	S	-0.09826846	15	5	0.01798	0.00508	-
			X	-0.09654257	15	6	0.02667	0.00743	-	
0.00042			Y	0.04031277	15	7	-0.01402	-0.20173		
0.01153			Z	-0.00005644	15	8	0.00001	0.00000		
0.00000										
0.18218			3	S	0.10575910	15	9	-0.27717	3.18811	-
			X	0.22002538	15	10	-0.33818	3.33999	-	
0.19086			Y	0.02691901	15	11	-0.11873	-0.03342		
0.00191			Z	-0.00004269	15	12	0.00002	0.00015	-	
0.00001										
0.00000			4	S	0.01233604	15	13	0.02502	0.00000	
			X	-0.37119618	15	14	0.06764	0.00000		
0.00000			Y	0.09744830	15	15	0.96092	0.00000		
1.00000			Z	-0.00018951	15	16	0.00003	0.00000		
0.00000										
0.36693			5	S	0.11899438	15	17	0.48830	-6.42136	
			X	0.14208178	15	18	0.00652	-0.26160		
0.01495			Y	-0.04921618	15	19	-0.62824	5.75740	-	
0.32899			Z	-0.00004089	15	20	0.00007	-0.00038		
0.00002										
0.06137			6	S	-0.14611761	15	21	-0.03036	-1.07401	
			X	0.03219991	15	22	-0.02882	-0.79199		
0.04526			Y	0.13938095	15	23	-0.00231	1.16582	-	
0.06662			Z	-0.00004903	15	24	0.00000	-0.00010		
0.00001										
0.06299			7	S	-0.07760397	15	25	0.02195	1.10237	-
			X	0.03275302	15	26	-0.01488	0.80108	-	
0.04578			Y	0.07778922	15	27	0.01685	1.20137	-	
0.06865			Z	0.00003179	15	28	-0.00003	0.00006		
0.00000										
0.00124			8	S	0.19781369	15	29	-0.01099	0.03884	-
			X	-0.15534189	15	30	-0.01119	0.03239	-	
0.00104			Y	-0.13667038	15	31	-0.02542	0.03700	-	
0.00118			Z	0.00013922	15	32	0.00002	-0.00001		
0.00000										

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00019		9	S	0.07311366	15	33	-0.00531	0.00608	-
			X	-0.11646484	15	34	-0.02255	0.00803	-
0.00026			Y	0.20407042	15	35	-0.00047	-0.00096	
0.00003			Z	-0.00010005	15	36	0.00000	0.00000	
0.00000		10	S	0.08806389	15	37	0.01920	-0.03329	
0.00107			X	-0.24431631	15	38	0.02092	-0.01479	
0.00047			Y	-0.04162440	15	39	-0.04166	0.03968	-
0.00127			Z	-0.00010764	15	40	0.00000	0.00000	
0.00000		11	S	0.00998846	15	41	-0.18223	4.05735	-
0.12984			X	0.39852616	15	42	0.31098	-3.90919	
0.12509			Y	-0.28148496	15	43	-0.11494	-0.04891	
0.00157			Z	-0.00036873	15	44	0.00005	-0.00064	
0.00002		12	S	-0.02409955	15	45	-0.00299	0.67044	-
0.03831			X	0.12414045	15	46	0.00379	-0.01570	
0.00090			Y	0.15336609	15	47	-0.02304	0.91510	-
0.05229			Z	-0.00003995	15	48	-0.00001	0.00035	-
0.00002		13	S	-0.10349662	15	49	-0.00415	0.01870	-
0.00127		14	S	-0.14564684	15	50	0.00340	-0.04766	
0.00323		15	S	0.17043696	15	51	0.00333	-0.02979	
0.00202		16	S	0.13693163	15	52	-0.04678	-1.63551	
0.11088		17	S	0.12163668	15	53	0.01940	-0.05334	
0.00362		18	S	0.17096528	15	54	-0.02262	1.29329	-
0.08768		19	S	-0.07269395	15	55	-0.00035	0.12067	-
0.00818		20	S	-0.07263894	15	56	-0.00035	0.12079	-
0.00819									
16	A*	-18.248301	1	S	-0.03178956	16	1	-0.00002	0.00005
0.00000			X	0.21611451	16	2	0.00003	0.00007	
0.00000			Y	0.01567203	16	3	-0.00001	-0.00004	
0.00000			Z	-0.00000577	16	4	-0.31723	-0.08610	
0.00492		2	S	0.01269737	16	5	0.00001	0.00011	-
0.00001			X	-0.02483943	16	6	0.00001	0.00016	-
0.00001			Y	-0.05218092	16	7	0.00000	0.00000	
0.00000			Z	-0.00004955	16	8	-0.04140	-0.20176	
0.01153		3	S	-0.13540317	16	9	0.00000	0.00025	-
0.00001			X	-0.12643878	16	10	-0.00008	0.00026	-
0.00001			Y	-0.06400023	16	11	0.00000	0.00015	-
0.00001			Z	-0.00008524	16	12	0.60934	-1.96027	
0.11202		4	S	-0.05747030	16	13	-0.00003	0.00000	
0.00000			X	0.07992528	16	14	0.00001	0.00000	
0.00000			Y	0.20325029	16	15	0.00003	0.00000	
0.00000			Z	-0.00015009	16	16	0.92563	0.00000	
1.00000		5	S	0.11599942	16	17	-0.00005	0.00032	-
0.00002			X	-0.03226229	16	18	-0.00006	0.00001	
0.00000			Y	-0.13459456	16	19	0.00003	-0.00038	
0.00002			Z	-0.00006263	16	20	0.67332	-1.98569	
0.11347									



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		6	S	-0.02472179	16	21	0.00001	0.00008	
			X	-0.12079262	16	22	0.00000	0.00006	
0.00000			Y	-0.23774311	16	23	-0.00001	-0.00010	
0.00001			Z	-0.00005897	16	24	0.03920	-0.19398	
0.01108		7	S	0.12193096	16	25	0.00001	0.00005	
0.00000			X	-0.08551264	16	26	0.00009	0.00003	
0.00000			Y	-0.04909587	16	27	-0.00002	0.00006	
0.00000			Z	-0.00002060	16	28	0.10001	-0.19928	
0.01139		8	S	-0.15427187	16	29	-0.00001	-0.00001	
0.00000			X	0.19185728	16	30	-0.00010	-0.00001	
0.00000			Y	0.16374326	16	31	-0.00001	-0.00001	
0.00000			Z	-0.00013542	16	32	-0.13555	-0.00360	
0.00012		9	S	0.00959880	16	33	-0.00001	0.00000	
0.00000			X	0.05835207	16	34	-0.00001	0.00000	
0.00000			Y	0.02750835	16	35	0.00001	0.00000	
0.00000			Z	-0.00007985	16	36	0.00236	-0.00240	
0.00008		10	S	0.23284850	16	37	0.00000	0.00000	
0.00000			X	-0.48558447	16	38	0.00000	0.00000	
0.00000			Y	0.38788891	16	39	0.00000	0.00000	
0.00000			Z	-0.00018987	16	40	-0.02102	-0.00247	
0.00008		11	S	0.06131588	16	41	0.00006	-0.00137	
0.00004			X	-0.04574263	16	42	-0.00011	0.00132	-
0.00004			Y	-0.26130778	16	43	0.00006	-0.00064	
0.00002			Z	-0.00042742	16	44	0.18981	-1.93374	
0.06188		12	S	-0.04639202	16	45	0.00004	0.00023	-
0.00001			X	0.03003643	16	46	-0.00001	-0.00001	
0.00000			Y	0.14985724	16	47	0.00003	0.00035	-
0.00002			Z	-0.00005657	16	48	-0.01718	-0.09094	
0.00520		13	S	-0.03270042	16	49	0.00001	0.00000	
0.00000		14	S	-0.14997514	16	50	0.00000	0.00000	
0.00000		15	S	-0.15285328	16	51	0.00001	0.00001	
0.00000		16	S	-0.02513999	16	52	0.00001	-0.00005	
0.00001		17	S	-0.13052836	16	53	-0.00001	-0.00013	
0.00006		18	S	0.12942751	16	54	-0.00003	0.00092	-
0.00202		19	S	-0.09232250	16	55	0.01989	0.02972	-
0.00201		20	S	-0.09237641	16	56	-0.01992	-0.02968	
	17 AP			-17.634005					
0.06256		1	S	0.00002435	17	1	-0.01006	-1.09480	
			X	-0.00005712	17	2	-0.02160	-1.46076	
0.08347			Y	-0.00025745	17	3	-0.01059	-0.00671	
0.00038			Z	0.04136794	17	4	-0.00001	-0.00010	
0.00001		2	S	0.00008003	17	5	-0.01570	-0.47077	
0.02690			X	0.00025643	17	6	0.00160	-0.56610	
0.03235			Y	0.00025132	17	7	-0.00073	-0.33287	
0.01902			Z	0.08259256	17	8	0.00002	-0.00003	
0.00000									

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.05868	3	S	0.00003668	17	9	-0.01342	-1.02686	
		X	-0.00007140	17	10	-0.02293	-0.66957	
0.03826		Y	0.00013297	17	11	-0.01196	-1.20180	
0.06867		Z	0.15875520	17	12	0.00001	0.00001	
0.00000	4	S	-0.00013229	17	13	0.31042	-6.00443	
0.34311		X	-0.00006103	17	14	0.01015	0.21694	-
0.01240		Y	-0.00007593	17	15	0.48830	-6.42136	
0.36693		Z	0.14720015	17	16	-0.00005	0.00032	-
0.00002	5	S	0.00009216	17	17	1.09488	0.00000	
1.00000		X	0.00024111	17	18	0.03132	0.00000	
0.00000		Y	0.00019259	17	19	0.01718	0.00000	
0.00000		Z	0.06176411	17	20	-0.00004	0.00000	
0.00000	6	S	-0.00015222	17	21	0.31375	-6.05027	
0.34573		X	0.00005502	17	22	0.43225	-5.51571	
0.31518		Y	0.00010994	17	23	-0.21818	3.36440	-
0.19225		Z	0.04726490	17	24	0.00000	-0.00039	
0.00002	7	S	0.00005620	17	25	0.02757	-0.05517	
0.00315		X	0.00013914	17	26	0.00552	-0.02578	
0.00147		Y	-0.00016078	17	27	0.03128	-0.07779	
0.00445		Z	0.28874025	17	28	0.00000	0.00000	
0.00000	8	S	-0.00015617	17	29	-0.00248	-0.00106	
0.00003		X	0.00029939	17	30	-0.00674	-0.00065	
0.00002		Y	0.00008056	17	31	-0.01392	-0.00124	
0.00004		Z	0.18818624	17	32	0.00001	0.00000	
0.00000	9	S	0.00006951	17	33	0.00135	-0.00594	
0.00019		X	-0.00036035	17	34	0.00155	-0.00671	
0.00021		Y	-0.00017848	17	35	0.00097	-0.00379	
0.00012		Z	0.08623587	17	36	-0.00001	0.00000	
0.00000	10	S	0.00013191	17	37	-0.00090	-0.70052	
0.02242		X	-0.00037591	17	38	-0.04615	-0.39895	
0.01277		Y	0.00001032	17	39	0.03894	0.71455	-
0.02287		Z	0.06571862	17	40	0.00000	-0.00005	
0.00000	11	S	0.00014580	17	41	-0.00389	-0.76962	
0.02463		X	-0.00008041	17	42	0.01423	0.49210	-
0.01575		Y	-0.00036152	17	43	-0.05474	-0.74784	
0.02393		Z	0.31168985	17	44	0.00001	0.00010	
0.00000	12	S	-0.00000864	17	45	-0.00005	-0.01795	
0.00103		X	0.00027962	17	46	-0.00101	0.00059	-
0.00003		Y	-0.00017595	17	47	0.00235	-0.02719	
0.00155		Z	0.61248928	17	48	0.00000	-0.00001	
0.00000	13	S	0.00010699	17	49	0.00056	-0.00619	
0.00042	14	S	-0.00019411	17	50	-0.00991	-0.64708	
0.04387	15	S	-0.00005168	17	51	0.04283	-0.13178	
0.00893	16	S	0.00029796	17	52	0.55595	-7.57107	
0.51329	17	S	-0.00016844	17	53	-0.01138	-0.58820	
0.03988								

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00477		18	S	-0.00017361	17	54	0.01166	-0.07038		
		19	S	-0.40963468	17	55	-0.00082	-0.00435		
0.00029		20	S	0.40976974	17	56	-0.00082	-0.00435		
0.00030										
0.08347	18 A*	-17.396650	1	S	0.02009555	18	1	0.01851	1.46076	-
				X	-0.01256583	18	2	0.00276	1.88554	-
0.10775				Y	-0.35490489	18	3	0.02682	0.00975	-
0.00056				Z	-0.00002290	18	4	0.00001	0.00014	-
0.00001			2	S	0.10417554	18	5	0.00158	0.56610	-
0.03235				X	0.29364944	18	6	-0.01379	0.64415	-
0.03681				Y	0.33857331	18	7	-0.00733	0.43092	-
0.02462				Z	-0.00003209	18	8	0.00003	0.00004	-
0.00000			3	S	-0.00307658	18	9	0.00081	0.66957	-
0.03826				X	-0.06427357	18	10	-0.00126	0.25476	-
0.01456				Y	0.13553217	18	11	-0.02344	0.85283	-
0.04873				Z	-0.00014899	18	12	0.00000	-0.00001	-
0.00000			4	S	-0.08536567	18	13	0.00814	-0.21694	-
0.01240				X	0.04042308	18	14	0.07609	-1.97686	-
0.11296				Y	-0.11331227	18	15	0.00652	-0.26160	-
0.01495				Z	-0.00004306	18	16	-0.00006	0.00001	-
0.00000			5	S	0.00154356	18	17	0.03132	0.00000	-
0.00000				X	0.18570754	18	18	0.95045	0.00000	-
1.00000				Y	0.16553295	18	19	0.02957	0.00000	-
0.00000				Z	-0.00002238	18	20	-0.00001	0.00000	-
0.00000			6	S	-0.10156217	18	21	-0.43384	5.51571	-
0.31518				X	0.08071158	18	22	-0.46229	3.66408	-
0.20938				Y	0.17760633	18	23	0.27994	-3.45863	-
0.19764				Z	-0.00006939	18	24	-0.00010	0.00040	-
0.00002			7	S	0.06481437	18	25	-0.00582	0.02578	-
0.00147				X	0.06954896	18	26	0.00068	0.00483	-
0.00028				Y	-0.17199750	18	27	-0.00423	0.03840	-
0.00219				Z	-0.00035140	18	28	0.00001	0.00000	-
0.00000			8	S	-0.08503489	18	29	0.00043	0.00083	-
0.00003				X	0.17132466	18	30	0.00018	0.00043	-
0.00001				Y	-0.03390615	18	31	0.00035	0.00100	-
0.00003				Z	-0.00032003	18	32	0.00000	0.00000	-
0.00000			9	S	0.10156305	18	33	-0.00167	0.00863	-
0.00028				X	-0.46008906	18	34	-0.00238	0.00957	-
0.00031				Y	-0.15366161	18	35	0.00024	0.00575	-
0.00018				Z	-0.00001526	18	36	-0.00001	0.00000	-
0.00000			10	S	0.04797775	18	37	-0.00783	0.53447	-
0.01710				X	-0.14594853	18	38	0.01024	0.20638	-
0.00660				Y	-0.15234295	18	39	-0.04920	-0.58863	-
0.01884				Z	-0.00021591	18	40	0.00001	0.00004	-
0.00000			11	S	0.04512693	18	41	-0.01397	-0.66031	-
0.02113										

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.01024			X	-0.09096801	18	42	-0.00599	0.32011	-
			Y	-0.07772556	18	43	-0.00154	-0.69359	
0.02220			Z	0.00001726	18	44	0.00001	0.00010	
0.00000									
0.00003		12	S	-0.03840355	18	45	-0.00127	-0.00059	
			X	-0.15299931	18	46	-0.00225	-0.00228	
0.00013			Y	0.07338103	18	47	-0.00087	-0.00094	
0.00005			Z	-0.00052118	18	48	0.00000	0.00000	
0.00000									
0.00044		13	S	0.08080634	18	49	-0.00228	0.00653	-
0.00556		14	S	-0.12501666	18	50	0.01836	0.08195	-
0.01190		15	S	-0.12004412	18	51	-0.04497	0.17547	-
0.41838		16	S	0.20051223	18	52	0.70843	-6.17109	
0.04394		17	S	-0.07159635	18	53	0.02215	-0.64806	
0.00151		18	S	-0.03717754	18	54	0.00219	-0.02230	
0.00002		19	S	-0.06497195	18	55	0.00044	-0.00023	
0.00002		20	S	-0.06581663	18	56	0.00044	-0.00023	
19 AP	-16.876434								
0.00038		1	S	0.00001760	19	1	-0.01090	0.00671	-
			X	0.00000477	19	2	-0.02827	0.00975	-
0.00056			Y	-0.00013519	19	3	-0.00359	-0.23772	
0.01358			Z	-0.08276045	19	4	0.00000	0.00000	
0.00000									
0.01902		2	S	0.00006541	19	5	-0.00004	0.33287	-
			X	0.00018622	19	6	-0.00886	0.43092	-
0.02462			Y	0.00011663	19	7	-0.00426	0.16470	-
0.00941			Z	-0.07660247	19	8	-0.00001	0.00002	
0.00000									
0.06867		3	S	-0.00008123	19	9	0.02918	1.20180	-
			X	-0.00013328	19	10	0.03342	0.85283	-
0.04873			Y	0.00008006	19	11	0.00140	1.31033	-
0.07488			Z	-0.07622908	19	12	0.00000	-0.00001	
0.00000									
0.36693		4	S	0.00009885	19	13	-0.49649	6.42136	-
			X	0.00017311	19	14	-0.00674	-0.26160	
0.01495			Y	0.00010619	19	15	-0.62824	5.75740	-
0.32899			Z	-0.24309196	19	16	0.00003	-0.00038	
0.00002									
0.00000		5	S	-0.00013560	19	17	0.01718	0.00000	
			X	0.00001147	19	18	0.02957	0.00000	
0.00000			Y	-0.00019922	19	19	0.91365	0.00000	
1.00000			Z	-0.13954030	19	20	0.00000	0.00000	
0.00000									
0.19225		6	S	0.00001068	19	21	0.25610	-3.36440	
			X	-0.00001715	19	22	0.31111	-3.45863	
0.19764			Y	0.00023624	19	23	-0.08559	0.10354	-
0.00592			Z	-0.17473902	19	24	0.00004	-0.00024	
0.00001									
0.00445		7	S	0.00007514	19	25	-0.03567	0.07779	-
			X	-0.00009853	19	26	-0.00505	0.03840	-
0.00219			Y	-0.00014750	19	27	-0.03454	0.10796	-
0.00617			Z	0.08227127	19	28	0.00001	0.00000	
0.00000									
0.00005		8	S	-0.00018772	19	29	0.00370	0.00158	-

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00003		X	0.00030409	19	30	0.00949	0.00100	-	
		Y	0.00021910	19	31	0.01483	0.00182	-	
0.00006		Z	0.06176879	19	32	-0.00002	0.00000		
0.00000									
0.00016		9	S	0.00004082	19	33	-0.00291	0.00487	-
		X	-0.00018007	19	34	0.00086	0.00575	-	
0.00018		Y	-0.00016037	19	35	-0.00345	0.00263	-	
0.00008		Z	-0.10485902	19	36	0.00000	0.00000		
0.00000									
0.03063		10	S	-0.00016027	19	37	-0.01220	-0.95729	
		X	0.00055037	19	38	-0.01119	-0.58863		
0.01884		Y	-0.00041757	19	39	0.02661	0.93205	-	
0.02983		Z	-0.41725445	19	40	-0.00001	-0.00008		
0.00000									
0.03211		11	S	-0.00020591	19	41	-0.00063	1.00346	-
		X	0.00004478	19	42	-0.04185	-0.69359		
0.02220		Y	0.00040102	19	43	0.02746	0.91775	-	
0.02937		Z	-0.73836279	19	44	-0.00001	-0.00015		
0.00000									
0.00155		12	S	-0.00003200	19	45	-0.00386	0.02719	-
		X	0.00023358	19	46	-0.00537	-0.00094		
0.00005		Y	0.00008901	19	47	-0.00607	0.04092	-	
0.00234		Z	0.26090112	19	48	0.00000	0.00001		
0.00000									
0.00039		13	S	0.00004779	19	49	0.00187	0.00570	-
		14	S	0.00012645	19	50	0.01284	-0.82799	
0.05614		15	S	-0.00004141	19	51	0.01669	-0.02622	
0.00178		16	S	-0.00015331	19	52	0.41265	-3.63262	
0.24628		17	S	0.00017535	19	53	0.01056	0.39552	-
0.02682		18	S	0.00015508	19	54	-0.01334	0.09321	-
0.00632		19	S	-0.17816627	19	55	0.00239	0.00601	-
0.00041		20	S	0.17804162	19	56	0.00238	0.00601	-
0.00041									
	20	A*	-16.765265	1	S	0.00156975	0.00010	-	
0.00001		X	0.15033476	20	2	0.00000	0.00014	-	
		Y	-0.13090724	20	3	0.00000	0.00000		
0.00000		Z	-0.00006502	20	4	-0.01429	-0.23776		
0.01359									
0.00000		2	S	0.07773957	20	5	0.00000	0.00003	
		X	-0.09446985	20	6	0.00002	0.00004		
0.00000		Y	0.08847250	20	7	-0.00001	0.00002		
0.00000		Z	-0.00005350	20	8	-0.30391	-0.08869		
0.00507									
0.00000		3	S	-0.03738723	20	9	0.00000	-0.00001	
		X	0.06070703	20	10	0.00001	-0.00001		
0.00000		Y	-0.10429247	20	11	0.00000	-0.00001		
0.00000		Z	-0.00009936	20	12	-0.05826	-0.22039		
0.01259									
0.00002		4	S	-0.07673618	20	13	0.00001	-0.00032	
		X	0.08446193	20	14	-0.00007	0.00001		
0.00000		Y	-0.11955142	20	15	0.00007	-0.00038		
0.00002		Z	-0.00004366	20	16	0.67332	-1.98569		
0.11347									
0.00000		5	S	0.00065518	20	17	-0.00004	0.00000	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		X	-0.01368664	20	18	-0.00001	0.00000			
0.00000		Y	0.14217794	20	19	0.00000	0.00000			
1.00000		Z	-0.00009935	20	20	1.10317	0.00000			
0.00002	6	S	0.03829018	20	21	-0.00002	0.00039	-		
0.00002		X	0.01329193	20	22	-0.00008	0.00040	-		
0.00001		Y	-0.12507549	20	23	0.00004	-0.00024			
0.11463		Z	-0.00022672	20	24	0.63855	-2.00610			
0.00000	7	S	0.00696804	20	25	0.00001	0.00000			
0.00000		X	0.40719455	20	26	-0.00002	0.00000			
0.00000		Y	0.08758768	20	27	0.00000	0.00000			
0.00045		Z	-0.00019481	20	28	-0.04006	-0.00790			
0.00000	8	S	0.25118858	20	29	0.00000	0.00000			
0.00000		X	-0.38160503	20	30	0.00001	0.00000			
0.00000		Y	-0.37060145	20	31	0.00000	0.00000			
0.00000		Z	0.00021192	20	32	0.02232	-0.00010			
0.00000	9	S	-0.08699480	20	33	-0.00001	0.00000			
0.00000		X	0.19307348	20	34	-0.00001	0.00000			
0.00000		Y	-0.08087689	20	35	0.00001	0.00000			
0.00002		Z	0.00011194	20	36	0.07336	-0.00061			
0.00000	10	S	0.08243960	20	37	0.00000	0.00007			
0.00000		X	-0.21004763	20	38	0.00002	0.00004			
0.00000		Y	0.16687769	20	39	0.00000	-0.00008			
0.00391		Z	-0.00074974	20	40	-0.11030	-0.12226			
0.00000	11	S	-0.06151058	20	41	-0.00001	-0.00014			
0.00000		X	-0.03309684	20	42	0.00001	0.00010			
0.00000		Y	0.23463061	20	43	-0.00001	-0.00015			
0.00436		Z	0.00002682	20	44	-0.11231	-0.13630			
0.00000	12	S	0.03234254	20	45	0.00000	0.00001			
0.00000		X	-0.20893325	20	46	0.00000	0.00000			
0.00000		Y	0.19303171	20	47	0.00000	0.00001			
0.00013		Z	0.00034677	20	48	0.00253	-0.00230			
0.00000	13	S	0.07305894	20	49	0.00001	0.00000			
0.00000	14	S	-0.07164620	20	50	-0.00001	-0.00004			
0.00000	15	S	-0.16214252	20	51	0.00000	0.00002			
0.00006	16	S	0.05277504	20	52	0.00010	-0.00093			
0.00000	17	S	0.07776434	20	53	0.00001	-0.00007			
0.00000	18	S	-0.05807604	20	54	0.00002	0.00004			
0.00007	19	S	-0.08930637	20	55	-0.00340	0.00104	-		
0.00007	20	S	-0.08902514	20	56	0.00340	-0.00104			
0.34580	21	AP	-16.606995	1	S	0.00000011	21	1	0.31473	-6.05141
0.31344		X	-0.00015635	21	2	0.43498	-5.48513			
0.19518		Y	0.00025996	21	3	0.26281	-3.41571			
0.00002		Z	-0.10169613	21	4	0.00004	-0.00034			
0.05351	2	S	-0.00015722	21	5	-0.02731	-0.93642			

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.03544		X	0.00000654	21	6	-0.00135	-0.62024	
		Y	-0.00019423	21	7	-0.03014	-1.09869	
0.06278		Z	-0.05841960	21	8	-0.00001	-0.00003	
0.00000	3	S	0.00016020	21	9	-0.01473	-0.42341	
0.02420		X	0.00001770	21	10	0.00175	0.00409	-
0.00023		Y	-0.00001227	21	11	-0.00005	-0.59326	
0.03390		Z	0.00219065	21	12	-0.00001	0.00002	
0.00000	4	S	-0.00001720	21	13	-0.02796	-0.92162	
0.05266		X	-0.00012286	21	14	-0.00027	0.62554	-
0.03575		Y	-0.00008036	21	15	-0.03036	-1.07401	
0.06137		Z	0.09577797	21	16	0.00001	0.00008	
0.00000	5	S	0.00007416	21	17	0.31375	-6.05027	
0.34573		X	-0.00005781	21	18	-0.43384	5.51571	-
0.31518		Y	0.00011471	21	19	0.25610	-3.36440	
0.19225		Z	-0.05176335	21	20	-0.00002	0.00039	-
0.00002	6	S	-0.00002094	21	21	1.11302	0.00000	
1.00000		X	0.00009548	21	22	-0.00535	0.00000	
0.00000		Y	-0.00015007	21	23	-0.06532	0.00000	
0.00000		Z	-0.24808012	21	24	0.00001	0.00000	
0.00000	7	S	-0.00010757	21	25	0.00327	-0.01462	
0.00084		X	-0.00036236	21	26	-0.00065	0.00012	-
0.00001		Y	0.00012621	21	27	0.00489	-0.02222	
0.00127		Z	-0.02490715	21	28	0.00000	0.00000	
0.00000	8	S	-0.00007030	21	29	0.00160	-0.00045	
0.00001		X	0.00008070	21	30	-0.00261	-0.00012	
0.00000		Y	0.00021466	21	31	0.00220	-0.00058	
0.00002		Z	-0.02005771	21	32	0.00000	0.00000	
0.00000	9	S	0.00009469	21	33	0.02236	-0.02324	
0.00074		X	-0.00012630	21	34	0.03324	-0.01962	
0.00063		Y	0.00019894	21	35	0.02612	-0.02222	
0.00071		Z	-0.09740456	21	36	0.00001	0.00000	
0.00000	10	S	0.00005021	21	37	0.20869	-6.95954	
0.22271		X	0.00009297	21	38	0.01059	-0.02004	
0.00064		Y	0.00018816	21	39	-0.46957	6.57301	-
0.21034		Z	-0.81361139	21	40	0.00003	-0.00033	
0.00001	11	S	0.00017889	21	41	0.01683	-0.02316	
0.00074		X	-0.00007080	21	42	-0.02908	0.01997	-
0.00064		Y	-0.00032530	21	43	0.03824	-0.02176	
0.00070		Z	0.48352081	21	44	-0.00001	0.00000	
0.00000	12	S	0.00000785	21	45	0.00210	-0.00181	
0.00010		X	0.00016421	21	46	0.00232	0.00071	-
0.00004		Y	-0.00043827	21	47	0.00241	-0.00273	
0.00016		Z	-0.05805609	21	48	0.00000	0.00000	
0.00000	13	S	-0.00014517	21	49	-0.01399	-0.01011	
0.00069	14	S	-0.00002060	21	50	-0.00212	-1.65306	
0.11207								

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.09883		15	S	0.00023897	21	51	-0.01562	-1.45775		
		16	S	0.00003339	21	52	-0.01405	-1.46669		
0.09944		17	S	-0.00016500	21	53	0.00441	-0.03143		
0.00213		18	S	-0.00014878	21	54	-0.00191	-0.00624		
0.00042		19	S	0.04027099	21	55	0.00001	-0.00056		
0.00004		20	S	-0.03980276	21	56	0.00001	-0.00056		
0.00004										
0.31344	22 A*	-16.451321	1	S	-0.00132049	22	1	-0.42631	5.48513	-
				X	-0.13833645	22	2	-0.45606	3.59983	-
0.20570				Y	-0.04209052	22	3	-0.31567	3.49125	-
0.19950				Z	0.00000415	22	4	-0.00007	0.00035	-
0.00002			2	S	0.07574563	22	5	0.02026	0.62024	-
0.03544				X	-0.09468815	22	6	-0.00638	0.24878	-
0.01422				Y	-0.00228731	22	7	0.02809	0.79082	-
0.04519				Z	0.00015107	22	8	-0.00001	0.00002	-
0.00000										
0.00023			3	S	-0.14743772	22	9	0.00166	-0.00409	-
0.00448				X	0.07439286	22	10	0.00124	-0.07845	-
0.00035				Y	0.15059823	22	11	0.00062	-0.00616	-
0.00000				Z	0.00000030	22	12	0.00001	0.00000	-
0.03575			4	S	0.08710508	22	13	-0.02366	-0.62554	-
0.01527				X	-0.12226074	22	14	-0.00675	0.26730	-
0.04526				Y	0.12955780	22	15	-0.02882	-0.79199	-
0.00000				Z	0.00004178	22	16	0.00000	0.00006	-
0.31518			5	S	0.01160974	22	17	0.43225	-5.51571	-
0.20938				X	-0.04139771	22	18	-0.46229	3.66408	-
0.19764				Y	-0.16052975	22	19	0.31111	-3.45863	-
0.00002				Z	-0.00001820	22	20	-0.00008	0.00040	-
0.00000			6	S	-0.04736383	22	21	-0.00535	0.00000	-
1.00000				X	0.05771620	22	22	1.00169	0.00000	-
0.00000				Y	0.14634503	22	23	0.00226	0.00000	-
0.00000				Z	-0.00009910	22	24	0.00003	0.00000	-
0.00001			7	S	0.08669155	22	25	-0.00080	-0.00012	-
0.00010				X	0.15969709	22	26	-0.00237	-0.00184	-
0.00001				Y	-0.26990435	22	27	0.00009	-0.00019	-
0.00000				Z	-0.00019711	22	28	0.00001	0.00000	-
0.00000			8	S	-0.11073087	22	29	-0.00113	0.00015	-
0.00000				X	0.16652305	22	30	0.00397	0.00000	-
0.00001				Y	-0.02158944	22	31	-0.00048	0.00021	-
0.00000				Z	-0.00024272	22	32	-0.00001	0.00000	-
0.00081			9	S	-0.18005598	22	33	-0.01976	0.02540	-
0.00063				X	0.44443083	22	34	-0.02323	0.01983	-
0.00082				Y	-0.37395597	22	35	-0.01959	0.02553	-
0.00000				Z	0.00069323	22	36	0.00000	0.00000	-
0.00092			10	S	-0.03840899	22	37	-0.00293	0.02877	-
0.06281				X	0.11666497	22	38	0.06419	-1.96291	-



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00098		Y	-0.18296430	22	39	-0.00011	-0.03072		
0.00000		Z	-0.00038547	22	40	-0.00001	0.00000		
0.00083		11 S	0.04636323	22	41	0.01595	-0.02586		
0.00066		X	0.09758303	22	42	-0.02076	0.02075	-	
0.00082		Y	-0.21691580	22	43	0.03271	-0.02554		
0.00000		Z	0.00036503	22	44	-0.00001	0.00000		
0.00004		12 S	-0.03527189	22	45	0.00120	-0.00071		
0.00001		X	-0.22056283	22	46	0.00401	0.00010	-	
0.00006		Y	0.21823591	22	47	0.00055	-0.00112		
0.00000		Z	0.00010115	22	48	0.00000	0.00000		
0.00050		13 S	0.20766437	22	49	0.01381	0.00737	-	
0.06462		14 S	0.01248855	22	50	0.01052	-0.95322		
0.12098		15 S	0.07643050	22	51	0.03763	1.78445	-	
0.12183		16 S	-0.09544098	22	52	-0.04000	-1.79697		
0.00251		17 S	-0.03425156	22	53	0.00241	-0.03696		
0.00026		18 S	0.01963452	22	54	-0.00225	-0.00379		
0.00001		19 S	-0.14102565	22	55	0.00016	-0.00019		
0.00001		20 S	-0.14109904	22	56	0.00016	-0.00019		
0.19518	23 AP	-15.974536	1 S	-0.00001786	23	1	-0.21915	3.41571	-
0.19950		X	0.00002156	23	2	-0.28127	3.49125	-	
0.00957		Y	-0.00021509	23	3	-0.09016	0.16747	-	
0.00001		Z	0.10733121	23	4	0.00001	0.00022	-	
0.06278		2 S	-0.00005281	23	5	0.01017	1.09869	-	
0.04519		X	-0.00017227	23	6	-0.01662	0.79082	-	
0.06875		Y	0.00025179	23	7	-0.00422	1.20320	-	
0.00000		Z	0.30678797	23	8	0.00001	0.00004		
0.03390		3 S	0.00000370	23	9	0.00002	0.59326	-	
0.00035		X	0.00011191	23	10	-0.00089	-0.00616		
0.04659		Y	-0.00023199	23	11	-0.01587	0.81526	-	
0.00000		Z	0.12098377	23	12	-0.00001	-0.00003		
0.06137		4 S	0.00002168	23	13	0.01227	1.07401	-	
0.04526		X	0.00004316	23	14	0.01726	-0.79199		
0.06662		Y	-0.00002723	23	15	-0.00231	1.16582	-	
0.00001		Z	0.01505328	23	16	-0.00001	-0.00010		
0.19225		5 S	-0.00001050	23	17	-0.21818	3.36440	-	
0.19764		X	-0.00017223	23	18	0.27994	-3.45863		
0.00592		Y	0.00000923	23	19	-0.08559	0.10354	-	
0.00001		Z	0.00509340	23	20	0.00004	-0.00024		
0.00000		6 S	0.00004532	23	21	-0.06532	0.00000		
0.00000		X	0.00014362	23	22	0.00226	0.00000		
1.00000		Y	-0.00003811	23	23	0.83387	0.00000		
0.00000		Z	-0.00758879	23	24	0.00000	0.00000		
0.00127		7 S	0.00000985	23	25	-0.00296	0.02222	-	
0.00001		X	-0.00026490	23	26	0.00023	-0.00019		

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00192		Y	0.00027131	23	27	-0.00261	0.03356	-
0.00000		Z	0.02099801	23	28	0.00000	0.00000	
0.00002	8	S	-0.00003102	23	29	-0.00076	0.00074	-
0.00001		X	-0.00011021	23	30	0.00121	0.00021	-
0.00003		Y	0.00037495	23	31	-0.00174	0.00096	-
0.00000		Z	0.01999926	23	32	0.00000	0.00000	
0.00092	9	S	0.00000541	23	33	-0.01376	0.02877	-
0.00082		X	-0.00035398	23	34	-0.01714	0.02553	-
0.00084		Y	0.00050472	23	35	-0.01117	0.02621	-
0.00000		Z	0.90122873	23	36	-0.00001	0.00000	
0.30194	10	S	0.00005680	23	37	0.40391	-9.43570	
0.00098		X	-0.00006758	23	38	0.02818	-0.03072	
0.25953		Y	0.00002060	23	39	-0.72928	8.11025	-
0.00002		Z	-0.20210351	23	40	0.00005	-0.00051	
0.00090	11	S	-0.00009753	23	41	-0.01191	0.02817	-
0.00082		X	0.00001882	23	42	0.01530	-0.02554	
0.00080		Y	0.00026017	23	43	-0.01754	0.02513	-
0.00000		Z	-0.12128416	23	44	0.00000	0.00000	
0.00016	12	S	0.00003015	23	45	-0.00128	0.00273	-
0.00006		X	0.00025572	23	46	-0.00069	-0.00112	
0.00023		Y	-0.00014204	23	47	-0.00175	0.00408	-
0.00000		Z	-0.07410678	23	48	0.00000	0.00000	
0.00081	13	S	-0.00003347	23	49	0.00604	0.01202	-
0.12072	14	S	-0.00007091	23	50	-0.01748	-1.78059	
0.01418	15	S	-0.00012654	23	51	0.02277	0.20918	-
0.01286	16	S	-0.00012994	23	52	0.02235	0.18967	-
0.00153	17	S	0.00011029	23	53	-0.00129	0.02255	-
0.00053	18	S	0.00007727	23	54	0.00050	0.00787	-
0.00005	19	S	0.05164052	23	55	0.00013	0.00077	-
0.00005	20	S	-0.05142730	23	56	0.00013	0.00077	-
0.00002	24	A*	-15.274868	1	S	-0.01558872	0.00034	-
0.00002		X	-0.06345719	24	2	-0.00011	0.00035	-
0.00001		Y	0.29665169	24	3	0.00000	0.00022	-
0.11466		Z	0.00001988	24	4	0.65548	-2.00661	
0.00000	2	S	-0.04049421	24	5	-0.00001	0.00003	
0.00000		X	0.06041902	24	6	-0.00001	0.00002	
0.00000		Y	-0.29060695	24	7	0.00000	0.00004	
0.01129		Z	0.00014413	24	8	0.07702	-0.19766	
0.00000	3	S	0.15095429	24	9	-0.00001	-0.00002	
0.00000		X	0.02680768	24	10	0.00003	0.00000	
0.00000		Y	0.23735674	24	11	-0.00001	-0.00003	
0.00449		Z	-0.00003244	24	12	-0.29986	-0.07849	
0.00000	4	S	-0.04199078	24	13	0.00002	-0.00008	
0.00000		X	-0.11557795	24	14	-0.00002	0.00006	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00001		Y	-0.29949093	24	15	0.00000	-0.00010			
		Z	-0.00022294	24	16	0.03920	-0.19398			
0.01108										
0.00002	5	S	0.00737227	24	17	0.00000	-0.00039			
		X	0.08390391	24	18	-0.00010	0.00040	-		
0.00002		Y	0.30985424	24	19	0.00004	-0.00024			
0.00001		Z	-0.00008273	24	20	0.63855	-2.00610			
0.11463										
0.00000	6	S	0.00876750	24	21	0.00001	0.00000			
		X	-0.01062407	24	22	0.00003	0.00000			
0.00000		Y	-0.14287637	24	23	0.00000	0.00000			
0.00000		Z	-0.00000576	24	24	0.90569	0.00000			
1.00000										
0.00000	7	S	-0.09052876	24	25	0.00000	0.00000			
		X	0.03713192	24	26	-0.00006	0.00000			
0.00000		Y	-0.19836260	24	27	0.00002	0.00000			
0.00000		Z	-0.00006707	24	28	-0.07407	-0.00184			
0.00010										
0.00000	8	S	-0.02118133	24	29	0.00000	0.00000			
		X	0.23097968	24	30	0.00007	0.00000			
0.00000		Y	-0.27156919	24	31	0.00000	0.00000			
0.00000		Z	-0.00019267	24	32	0.09634	-0.00004			
0.00000										
0.00000	9	S	0.02499902	24	33	0.00000	0.00000			
		X	0.10750286	24	34	0.00001	0.00000			
0.00000		Y	-0.02437722	24	35	-0.00002	0.00000			
0.00000		Z	0.00048719	24	36	-0.03344	-0.00271			
0.00009										
0.00002	10	S	0.01473188	24	37	-0.00003	0.00048	-		
		X	-0.11766554	24	38	-0.00003	0.00000			
0.00000		Y	0.22203048	24	39	0.00004	-0.00051			
0.00002		Z	0.00000430	24	40	0.19847	-1.96301			
0.06282										
0.00000	11	S	0.11528105	24	41	0.00000	0.00000			
		X	-0.05352305	24	42	0.00000	0.00000			
0.00000		Y	-0.15886082	24	43	0.00000	0.00000			
0.00000		Z	-0.00081521	24	44	-0.02089	-0.00270			
0.00009										
0.00000	12	S	-0.05920160	24	45	-0.00002	0.00000			
		X	-0.20342176	24	46	0.00002	0.00000			
0.00000		Y	-0.21004818	24	47	-0.00002	0.00000			
0.00000		Z	0.00009662	24	48	0.01358	-0.00019			
0.00001										
0.00000	13	S	-0.02926690	24	49	-0.00001	0.00000			
	14	S	-0.00345902	24	50	0.00001	-0.00020			
0.00001										
0.00001	15	S	0.16849454	24	51	-0.00001	0.00021	-		
	16	S	0.20700656	24	52	0.00001	-0.00019			
0.00001										
0.00000	17	S	-0.07894811	24	53	0.00000	0.00000			
	18	S	-0.20144591	24	54	-0.00001	0.00000			
0.00000										
0.00001	19	S	0.06203202	24	55	-0.01455	0.00012	-		
	20	S	0.06197010	24	56	0.01457	-0.00012			
0.00001										
	25	A*	-15.165573	1	S	0.00572004	25	1	0.02398	-0.05494
0.00314					X	0.21663581	25	2	0.00709	-0.02650
0.00151										

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00441		Y	0.22489698	25	3	-0.03192	0.07719	-
0.00000		Z	0.00007768	25	4	0.00000	0.00000	
0.05414	2	S	0.02969655	25	5	-0.00485	-0.94744	
0.03658		X	0.17867930	25	6	-0.02011	-0.64023	
0.06305		Y	-0.22948188	25	7	0.01575	1.10332	-
0.00000		Z	0.00018524	25	8	0.00000	-0.00006	
0.33216	3	S	0.01835966	25	9	0.29422	-5.81281	
0.00072		X	-0.26119754	25	10	0.00138	-0.01266	
0.35846		Y	0.06089850	25	11	-0.49272	6.27313	-
0.00001		Z	-0.00001251	25	12	0.00000	0.00017	-
0.05388	4	S	-0.03572248	25	13	-0.01371	-0.94295	
0.03603		X	0.09943263	25	14	0.02520	0.63048	-
0.06299		Y	0.21744291	25	15	0.02195	1.10237	-
0.00000		Z	0.00010021	25	16	0.00001	0.00005	
0.00315	5	S	-0.03676663	25	17	0.02757	-0.05517	
0.00147		X	0.26165867	25	18	-0.00582	0.02578	-
0.00445		Y	-0.20523587	25	19	-0.03567	0.07779	-
0.00000		Z	0.00006863	25	20	0.00001	0.00000	
0.00084	6	S	0.00517294	25	21	0.00327	-0.01462	
0.00001		X	-0.37959278	25	22	-0.00080	-0.00012	
0.00127		Y	0.04801768	25	23	-0.00296	0.02222	-
0.00000		Z	-0.00004409	25	24	0.00000	0.00000	
1.00000	7	S	0.00120686	25	25	1.13788	0.00000	
0.00000		X	0.17347389	25	26	0.04035	0.00000	
0.00000		Y	-0.06683721	25	27	0.01499	0.00000	
0.00000		Z	-0.00015649	25	28	-0.00001	0.00000	
0.29028	8	S	0.07953725	25	29	0.23757	-9.07111	
0.21359		X	0.01975446	25	30	0.40811	-6.67458	
0.14502		Y	-0.30761474	25	31	0.29483	-4.53188	
0.00011		Z	-0.00003345	25	32	-0.00019	0.00356	-
0.00741	9	S	0.09371987	25	33	-0.01021	-0.23168	
0.00777		X	-0.14999293	25	34	-0.01046	-0.24284	
0.00457		Y	0.13180813	25	35	-0.00315	0.14278	-
0.00000		Z	0.00046586	25	36	-0.00001	-0.00002	
0.00000	10	S	-0.09863115	25	37	0.00145	-0.00007	
0.00000		X	0.27080211	25	38	0.00132	0.00000	
0.00000		Y	-0.10366282	25	39	-0.00100	0.00010	
0.00000		Z	-0.00020264	25	40	0.00000	0.00000	
0.00680	11	S	-0.01874590	25	41	-0.00616	-0.21252	
0.00709		X	-0.00503440	25	42	0.01394	0.22168	-
0.00429		Y	-0.06967951	25	43	-0.01019	0.13404	-
0.00000		Z	0.00037442	25	44	0.00000	0.00003	
0.33634	12	S	0.01387954	25	45	0.25680	-5.88604	
0.32213		X	-0.05719084	25	46	-0.46078	5.63727	-
0.16473		Y	0.23512860	25	47	0.23366	-2.88278	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00022		Z	0.00009279	25	48	0.00032	-0.00392	
0.05415		13 S	-0.10896511	25	49	0.01143	-0.79877	
0.00002		14 S	0.13991819	25	50	-0.00055	-0.00023	
0.00059		15 S	-0.06570534	25	51	-0.01627	-0.00877	
0.00059		16 S	0.09446645	25	52	-0.01750	-0.00875	
0.00188		17 S	-0.03574134	25	53	-0.00236	-0.02776	
0.11197		18 S	0.11122346	25	54	-0.00541	-1.65149	
0.11196		19 S	-0.11670417	25	55	-0.00074	-1.65148	
0.11196		20 S	-0.11663098	25	56	-0.00074	-1.65146	
0.00151	26 A*							
			-13.957112					
0.00032		1 S	0.07170939	26	1	-0.00864	0.02650	-
0.00225		X	0.35966593	26	2	0.00043	0.00563	-
0.00000		Y	-0.07445259	26	3	0.00718	-0.03933	
0.03658		Z	0.00014101	26	4	-0.00001	0.00000	
0.01542		2 S	-0.01757686	26	5	0.01025	0.64023	-
0.04631		X	-0.20493801	26	6	0.00828	0.26983	-
0.00000		Y	0.13209222	26	7	0.01305	-0.81036	
0.00072		Z	0.00005680	26	8	0.00009	0.00004	
0.10864		3 S	-0.02252731	26	9	-0.03514	0.01266	-
0.00088		X	0.31340641	26	10	0.06551	-1.90115	
0.00000		Y	0.04626658	26	11	0.03462	-0.01539	
0.03603		Z	0.00027887	26	12	0.00014	0.00000	
0.01479		4 S	0.06071658	26	13	-0.00470	-0.63048	
0.04578		X	-0.18861027	26	14	-0.00012	0.25888	-
0.00000		Y	-0.20385276	26	15	-0.01488	0.80108	-
0.00147		Z	0.00015577	26	16	0.00009	0.00003	
0.00028		5 S	-0.10236491	26	17	0.00552	-0.02578	
0.00219		X	0.35152921	26	18	0.00068	0.00483	-
0.00000		Y	0.11319963	26	19	-0.00505	0.03840	-
0.00001		Z	0.00016684	26	20	-0.00002	0.00000	
0.00010		6 S	0.01555938	26	21	-0.00065	0.00012	-
0.00001		X	-0.35303870	26	22	-0.00237	-0.00184	
0.00000		Y	-0.00158642	26	23	0.00023	-0.00019	
0.00000		Z	0.00004835	26	24	-0.00006	0.00000	
0.00000		7 S	-0.02316173	26	25	0.04035	0.00000	
1.00000		X	-0.14352873	26	26	1.00595	0.00000	
0.00000		Y	-0.04458060	26	27	-0.02555	0.00000	
0.00000		Z	0.00030467	26	28	-0.00026	0.00000	
0.31193		8 S	-0.05197849	26	29	-0.35739	9.74792	-
0.17232		X	0.07541951	26	30	-0.46258	5.38503	-
0.17748		Y	0.21030371	26	31	-0.37962	5.54621	-
0.00014		Z	0.00020946	26	32	0.00072	-0.00435	
0.01026		9 S	-0.02835279	26	33	-0.00025	0.32049	-
0.01037		X	0.21268554	26	34	-0.00693	0.32391	-
0.00675		Y	-0.02523802	26	35	0.00233	-0.21082	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		Z	-0.00022457	26	36	-0.00003	0.00003		
0.00000		10	S	-0.03983284	26	37	-0.00001	0.00000	
0.00000		X	0.09105920	26	38	0.00032	-0.00001		
0.00000		Y	-0.02098760	26	39	-0.00044	0.00000		
0.00000		Z	-0.00013963	26	40	0.00002	0.00000		
0.00000		11	S	-0.06744453	26	41	0.00234	-0.29229	
0.00935		X	0.09743179	26	42	0.00131	0.29374	-	
0.00940		Y	0.03091240	26	43	-0.00399	0.19662	-	
0.00629		Z	-0.00000625	26	44	-0.00003	0.00004		
0.00000		12	S	-0.00643290	26	45	0.36878	-5.63727	
0.32213		X	0.11633003	26	46	-0.52977	4.15282	-	
0.23730		Y	-0.01312613	26	47	0.29575	-3.11233		
0.17785		Z	-0.00023993	26	48	0.00049	-0.00423		
0.00024		13	S	0.03053323	26	49	-0.01096	0.99927	-
0.06775		14	S	0.06183925	26	50	0.00033	-0.00005	
0.00000		15	S	-0.28943914	26	51	0.00308	0.00563	-
0.00038		16	S	0.29516625	26	52	0.00000	-0.00550	
0.00037		17	S	0.08352746	26	53	-0.00274	-0.03202	
0.00217		18	S	0.04829215	26	54	-0.00397	-2.01736	
0.13677		19	S	0.01275198	26	55	-0.00221	-1.36127	
0.09229		20	S	0.01251735	26	56	-0.00208	-1.36237	
0.09236									
27	AP		-13.212255	1	S	0.00005707	0.03346	-0.07719	
0.00441		X	0.00032024	27	2	0.00554	-0.03933		
0.00225		Y	-0.00014510	27	3	-0.03719	0.10670	-	
0.00610		Z	-0.21742792	27	4	0.00001	0.00000		
0.00000		2	S	-0.00005252	27	5	-0.02518	-1.10332	
0.06305		X	-0.00020676	27	6	-0.03851	-0.81036		
0.04631		Y	0.00020568	27	7	0.01513	1.19611	-	
0.06835		Z	-0.21404818	27	8	-0.00004	-0.00008		
0.00000		3	S	-0.00001467	27	9	0.47354	-6.27313	
0.35846		X	0.00026084	27	10	-0.00135	-0.01539		
0.00088		Y	-0.00021146	27	11	-0.63942	5.72907	-	
0.32738		Z	-0.41558650	27	12	-0.00002	0.00021	-	
0.00001		4	S	0.00006038	27	13	-0.01934	-1.10237	
0.06299		X	-0.00011278	27	14	0.03518	0.80108	-	
0.04578		Y	0.00001085	27	15	0.01685	1.20137	-	
0.06865		Z	-0.27623165	27	16	-0.00002	0.00006		
0.00000		5	S	-0.00000704	27	17	0.03128	-0.07779	
0.00445		X	0.00028375	27	18	-0.00423	0.03840	-	
0.00219		Y	-0.00008221	27	19	-0.03454	0.10796	-	
0.00617		Z	-0.25547755	27	20	0.00000	0.00000		
0.00000		6	S	-0.00001309	27	21	0.00489	-0.02222	
0.00127		X	-0.00028983	27	22	0.00009	-0.00019		
0.00001		Y	0.00003766	27	23	-0.00261	0.03356	-	
0.00192									

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		Z	-0.18569630	27	24	0.00002	0.00000	
0.00000		7	S	0.00002610	27	25	0.01499	0.00000
0.00000		X	-0.00026676	27	26	-0.02555	0.00000	
1.00000		Y	0.00024193	27	27	0.98593	0.00000	
0.00000		Z	-0.32910565	27	28	0.00005	0.00000	
0.21180		8	S	0.00001644	27	29	-0.23730	6.61861 -
0.17748		X	-0.00051334	27	30	-0.36583	5.54621 -	
0.03143		Y	0.00029196	27	31	-0.13737	0.98229 -	
0.00009		Z	-0.47072941	27	32	0.00015	-0.00295	
0.00603		9	S	-0.00004432	27	33	-0.01151	-0.18844
0.00675		X	-0.00001038	27	34	-0.00415	-0.21082	
0.00286		Y	0.00024155	27	35	0.00112	0.08931 -	
0.00000		Z	0.27498153	27	36	0.00000	-0.00002	
0.00000		10	S	-0.00003160	27	37	0.00090	-0.00012
0.00000		X	0.00006454	27	38	0.00128	0.00000	
0.00001		Y	-0.00007209	27	39	0.00059	0.00017 -	
0.00000		Z	0.16433944	27	40	0.00000	0.00000	
0.00566		11	S	0.00018495	27	41	-0.00418	-0.17673
0.00629		X	0.00004048	27	42	0.00415	0.19662 -	
0.00280		Y	-0.00045035	27	43	-0.00606	0.08745 -	
0.00000		Z	0.20614365	27	44	0.00001	0.00002	
0.16473		12	S	-0.00009558	27	45	-0.20568	2.88278 -
0.17785		X	-0.00004306	27	46	0.30860	-3.11233	
0.01953		Y	-0.00051013	27	47	-0.09431	-0.34174	
0.00012		Z	0.19817325	27	48	-0.00022	0.00216 -	
0.01309		13	S	0.00001654	27	49	0.01186	-0.19305
0.00002		14	S	0.00005719	27	50	-0.00089	-0.00033
0.00074		15	S	-0.00026928	27	51	-0.02264	-0.01086
0.00074		16	S	0.00015905	27	52	-0.02207	-0.01091
0.00142		17	S	-0.00017509	27	53	-0.00335	-0.02101
0.00315		18	S	-0.00037736	27	54	0.00150	-0.04650
0.08376		19	S	-0.14785744	27	55	0.00029	1.23548 -
0.08376		20	S	0.14829126	27	56	0.00027	1.23550 -
0.00000	28	A*	-12.948923	1	S	-0.03406141	0.00002	0.00000
0.00000		X	-0.09733239	28	2	0.00001	0.00000	
0.00000		Y	0.08695712	28	3	-0.00003	0.00000	
0.00045		Z	-0.00019239	28	4	-0.02329	-0.00787	
0.00000		2	S	0.01590012	28	5	-0.00004	0.00006
0.00000		X	0.08078644	28	6	-0.00006	0.00004	
0.00000		Y	-0.11203390	28	7	0.00006	-0.00008	
0.01145		Z	-0.00017233	28	8	0.10467	-0.20040	
0.00001		3	S	0.00273088	28	9	0.00005	-0.00017
0.00000		X	-0.02234371	28	10	0.00005	0.00000	
0.00001		Y	0.19905822	28	11	-0.00006	0.00021 -	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.10864		Z	-0.00038368	28	12	0.32401	-1.90118	
0.00000	4	S	0.00340700	28	13	0.00002	-0.00005	
0.00000		X	0.00975094	28	14	-0.00004	0.00003	
0.00000		Y	-0.16937552	28	15	-0.00003	0.00006	
0.01139		Z	-0.00005742	28	16	0.10001	-0.19928	
0.00000	5	S	-0.04022520	28	17	0.00000	0.00000	
0.00000		X	-0.08236992	28	18	0.00001	0.00000	
0.00000		Y	0.15683502	28	19	0.00001	0.00000	
0.00045		Z	-0.00011817	28	20	-0.04006	-0.00790	
0.00000	6	S	0.02632306	28	21	0.00000	0.00000	
0.00000		X	0.11719196	28	22	0.00001	0.00000	
0.00000		Y	-0.05161205	28	23	0.00000	0.00000	
0.00010		Z	-0.00010435	28	24	-0.07407	-0.00184	
0.00000	7	S	-0.06953841	28	25	-0.00001	0.00000	
0.00000		X	-0.10007769	28	26	-0.00026	0.00000	
0.00000		Y	-0.18888183	28	27	0.00005	0.00000	
1.00000		Z	-0.00034777	28	28	0.57437	0.00000	
0.00017	8	S	-0.03481326	28	29	0.00019	-0.00519	
0.00014		X	0.23814683	28	30	0.00071	-0.00435	
0.00009		Y	0.00275024	28	31	0.00015	-0.00295	
0.08907		Z	-0.00076062	28	32	0.78928	-2.78345	
0.00000	9	S	0.01599371	28	33	0.00002	0.00003	
0.00000		X	-0.00363655	28	34	0.00003	0.00003	
0.00000		Y	-0.02829590	28	35	-0.00007	-0.00002	
0.00111		Z	0.00026656	28	36	-0.03402	-0.03464	
0.00000	10	S	0.00731530	28	37	0.00000	0.00000	
0.00000		X	-0.05862356	28	38	0.00000	0.00000	
0.00000		Y	0.07246819	28	39	0.00000	0.00000	
0.00000		Z	0.00009479	28	40	0.01993	-0.00001	
0.00000	11	S	-0.20326404	28	41	0.00000	-0.00004	
0.00000		X	-0.01076900	28	42	0.00000	0.00004	
0.00000		Y	0.45805246	28	43	-0.00001	0.00002	
0.00101		Z	0.00069439	28	44	-0.02893	-0.03144	
0.00022	12	S	0.08893006	28	45	-0.00025	0.00392	-
0.00024		X	0.29787260	28	46	0.00048	-0.00423	
0.00012		Y	0.40166360	28	47	-0.00021	0.00216	-
0.11048		Z	0.00011027	28	48	0.18895	-1.93332	
0.00001	13	S	-0.01174966	28	49	-0.00003	-0.00012	
0.00000	14	S	-0.01915560	28	50	0.00000	0.00000	
0.00000	15	S	0.10617070	28	51	-0.00001	0.00000	
0.00000	16	S	-0.00565596	28	52	0.00000	0.00000	
0.00000	17	S	0.20425965	28	53	0.00001	0.00000	
0.00009	18	S	0.34138337	28	54	-0.00001	0.00140	-
0.05641	19	S	-0.15172265	28	55	-0.11002	0.83212	-
0.05629	20	S	-0.15124619	28	56	0.11003	-0.83024	



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

29	AP	-12.286889	1	S	-0.00003018	29	1	-0.00137	-0.00541	
0.00017				X	0.00001657	29	2	0.00001	-0.00034	
0.00001				Y	0.00003870	29	3	0.00024	0.00902	-
0.00029				Z	-0.29901457	29	4	0.00000	0.00000	
0.00000			2	S	0.00003964	29	5	-0.00446	-0.26426	
0.00846				X	0.00008269	29	6	-0.00816	-0.02689	
0.00086				Y	-0.00007075	29	7	-0.00036	0.42219	-
0.01351				Z	-0.17784412	29	8	-0.00001	-0.00010	
0.00000			3	S	-0.00002055	29	9	0.01060	-0.84405	
0.02701				X	-0.00004362	29	10	0.00386	0.57770	-
0.01849				Y	0.00009330	29	11	-0.00836	1.17984	-
0.03775				Z	-0.11633330	29	12	0.00000	-0.00029	
0.00001			4	S	-0.00001430	29	13	0.01079	-0.03016	
0.00097				X	0.00004210	29	14	-0.00992	0.03099	-
0.00099				Y	-0.00004564	29	15	-0.01099	0.03884	-
0.00124				Z	-0.22165400	29	16	-0.00001	-0.00001	
0.00000			5	S	0.00001077	29	17	-0.00248	-0.00106	
0.00003				X	0.00002575	29	18	0.00043	0.00083	-
0.00003				Y	0.00003073	29	19	0.00370	0.00158	-
0.00005				Z	-0.33903566	29	20	0.00000	0.00000	
0.00000			6	S	-0.00000250	29	21	0.00160	-0.00045	
0.00001				X	0.00002681	29	22	-0.00113	0.00015	
0.00000				Y	-0.00002002	29	23	-0.00076	0.00074	-
0.00002				Z	-0.30422103	29	24	0.00000	0.00000	
0.00000			7	S	-0.00000576	29	25	0.23757	-9.07111	
0.29028				X	0.00018038	29	26	-0.35739	9.74792	-
0.31193				Y	-0.00010807	29	27	-0.23730	6.61861	-
0.21180				Z	0.29458380	29	28	0.00019	-0.00519	
0.00017			8	S	-0.00001716	29	29	1.75554	0.00000	
1.00000				X	0.00037503	29	30	-0.33479	0.00000	
0.00000				Y	0.00003541	29	31	-0.24683	0.00000	
0.00000				Z	0.64093506	29	32	0.00018	0.00000	
0.00000			9	S	0.00000779	29	33	-0.03778	-0.16636	
0.00370				X	0.00000559	29	34	-0.01438	-0.13591	
0.00302				Y	-0.00005631	29	35	0.06587	0.20540	-
0.00456				Z	0.13444801	29	36	-0.00003	-0.00007	
0.00000			10	S	-0.00000937	29	37	-0.00036	0.00000	
0.00000				X	-0.00004178	29	38	-0.00022	0.00000	
0.00000				Y	0.00002008	29	39	0.00076	0.00000	
0.00000				Z	0.19697048	29	40	0.00000	0.00000	
0.00000			11	S	-0.00002602	29	41	-0.00187	-0.00055	
0.00001				X	-0.00002813	29	42	-0.00211	0.00074	-
0.00002				Y	0.00009105	29	43	0.00131	0.00046	-
0.00001				Z	0.13626352	29	44	0.00001	0.00000	
0.00000										

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.03192		12	S	0.00003684	29	45	0.00610	-0.99739	
			X	-0.00004311	29	46	-0.00773	1.54326	-
0.04938			Y	0.00012494	29	47	0.00967	0.04525	-
0.00145			Z	-0.12950614	29	48	0.00001	-0.00096	
0.00003		13	S	0.00002048	29	49	0.09156	-2.77905	
0.09751		14	S	0.00001381	29	50	0.00014	-0.00001	
0.00000		15	S	0.00003976	29	51	-0.00039	-0.00213	
0.00007		16	S	0.00000127	29	52	0.00175	-0.00028	
0.00001		17	S	0.00002423	29	53	0.00263	-0.00074	
0.00003		18	S	0.00006840	29	54	0.02146	-0.12280	
0.00431		19	S	0.09745079	29	55	-0.00089	-0.44240	
0.01552		20	S	-0.09754363	29	56	-0.00089	-0.44232	
0.01552									
30	A*	-11.328595							
0.00001		1	S	-0.04606681	30	1	0.00689	0.00026	-
			X	-0.02164027	30	2	-0.00095	-0.00054	
0.00002			Y	0.11442270	30	3	-0.00379	-0.00046	
0.00001			Z	0.00008302	30	4	0.00000	0.00000	
0.00000		2	S	0.03913771	30	5	-0.01735	0.02034	-
0.00065			X	0.08127982	30	6	-0.00123	-0.03798	
0.00122			Y	-0.13979389	30	7	0.00830	-0.03473	
0.00111			Z	0.00003113	30	8	-0.00010	0.00001	
0.00000		3	S	-0.06387882	30	9	0.01252	-0.42985	
0.01376			X	-0.04742657	30	10	0.00115	0.16674	-
0.00534			Y	0.27137020	30	11	0.01030	0.65032	-
0.02081			Z	-0.00005940	30	12	-0.00004	-0.00016	
0.00001		4	S	0.01158930	30	13	0.01355	-0.02390	
0.00076			X	-0.03809119	30	14	-0.01130	0.02224	-
0.00071			Y	-0.07211098	30	15	-0.01119	0.03239	-
0.00104			Z	0.00001320	30	16	-0.00010	-0.00001	
0.00000		5	S	-0.02007555	30	17	-0.00674	-0.00065	
0.00002			X	0.01378556	30	18	0.00018	0.00043	-
0.00001			Y	0.06323745	30	19	0.00949	0.00100	-
0.00003			Z	0.00010472	30	20	0.00001	0.00000	
0.00000		6	S	0.00710203	30	21	-0.00261	-0.00012	
0.00000			X	-0.00850327	30	22	0.00397	0.00000	
0.00000			Y	-0.01651124	30	23	0.00121	0.00021	-
0.00001			Z	0.00011174	30	24	0.00007	0.00000	
0.00000		7	S	-0.00367857	30	25	0.40811	-6.67458	
0.21359			X	0.18294139	30	26	-0.46258	5.38503	-
0.17232			Y	-0.24771485	30	27	-0.36583	5.54621	-
0.17748			Z	-0.00016448	30	28	0.00071	-0.00435	
0.00014		8	S	0.01222430	30	29	-0.33479	0.00000	
0.00000			X	-0.46801463	30	30	1.47005	0.00000	
1.00000			Y	0.63899332	30	31	-0.33233	0.00000	
0.00000			Z	0.00033818	30	32	-0.00001	0.00000	
0.00000									

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00302		9	S	-0.00804792	30	33	0.05526	0.13591	-			
			X	-0.07757237	30	34	0.02091	0.09316	-			
0.00207			Y	0.19693783	30	35	-0.08897	-0.17745				
0.00394			Z	-0.00007809	30	36	0.00007	0.00006				
0.00000		10	S	-0.00751953	30	37	0.00031	0.00000				
0.00000			X	-0.00404576	30	38	-0.00057	0.00000				
0.00000			Y	0.02597419	30	39	-0.00051	0.00000				
0.00000			Z	-0.00006110	30	40	-0.00002	0.00000				
0.00000		11	S	0.02028017	30	41	-0.00492	-0.00074				
0.00002			X	-0.01399785	30	42	-0.00598	0.00098	-			
0.00002			Y	-0.00648441	30	43	0.00481	0.00064	-			
0.00001			Z	-0.00007218	30	44	0.00003	0.00000				
0.00000		12	S	0.07707904	30	45	-0.04615	-1.14482				
0.03663			X	-0.24845056	30	46	0.04813	1.73738	-			
0.05560			Y	0.11631296	30	47	-0.03286	0.05634	-			
0.00180			Z	0.00016788	30	48	-0.00008	-0.00119				
0.00004		13	S	-0.03275034	30	49	-0.14527	2.08650	-			
0.07321		14	S	0.00584200	30	50	-0.00058	0.00000				
0.00000		15	S	0.05756395	30	51	-0.00052	0.00050	-			
0.00002		16	S	0.03780587	30	52	0.00309	-0.00017				
0.00001		17	S	-0.00822844	30	53	0.00658	-0.00068				
0.00002		18	S	-0.06149220	30	54	0.05181	-0.13005				
0.00456		19	S	-0.05190784	30	55	0.00017	-0.43962				
0.01543		20	S	-0.05191093	30	56	0.00008	-0.43972				
0.01543												
	31	AP		-9.931761	1	S	0.00002509	31	1	-0.00493	-0.00702	
0.00022			X	-0.00005520	31	2	-0.00049	-0.00046				
0.00001			Y	0.00000216	31	3	0.00245	0.01168	-			
0.00037			Z	0.37980479	31	4	0.00000	0.00000				
0.00000		2	S	-0.00001301	31	5	0.00694	-0.31942				
0.01022			X	0.00000139	31	6	0.00038	-0.03473				
0.00111			Y	0.00000964	31	7	-0.01563	0.50513	-			
0.01616			Z	-0.12314261	31	8	0.00000	-0.00013				
0.00000		3	S	-0.00001075	31	9	-0.08240	-0.87789				
0.02809			X	0.00005650	31	10	-0.01048	0.65032	-			
0.02081			Y	-0.00004570	31	11	0.06917	1.17647	-			
0.03765			Z	-0.57364064	31	12	0.00002	-0.00032				
0.00001		4	S	0.00002563	31	13	0.03932	-0.02995				
0.00096			X	0.00002030	31	14	-0.03355	0.03239	-			
0.00104			Y	-0.00002668	31	15	-0.02542	0.03700	-			
0.00118			Z	-0.30557293	31	16	-0.00001	-0.00001				
0.00000		5	S	-0.00001659	31	17	-0.01392	-0.00124				
0.00004			X	-0.00002350	31	18	0.00035	0.00100	-			
0.00003			Y	0.00000952	31	19	0.01483	0.00182	-			
0.00006			Z	0.20628247	31	20	0.00000	0.00000				
0.00000												

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00002		6	S	0.00000865	31	21	0.00220	-0.00058	
			X	-0.00001158	31	22	-0.00048	0.00021	-
0.00001			Y	0.00001721	31	23	-0.00174	0.00096	-
0.00003			Z	0.47799087	31	24	0.00000	0.00000	
0.00000		7	S	-0.00000995	31	25	0.29483	-4.53188	
0.14502			X	-0.00010162	31	26	-0.37962	5.54621	-
0.17748			Y	0.00005023	31	27	-0.13737	0.98229	-
0.03143			Z	-0.02761696	31	28	0.00015	-0.00295	
0.00009		8	S	-0.00000453	31	29	-0.24683	0.00000	
0.00000			X	0.00026604	31	30	-0.33233	0.00000	
0.00000			Y	-0.00004918	31	31	1.73388	0.00000	
1.00000			Z	0.31146714	31	32	0.00021	0.00000	
0.00000		9	S	0.00000633	31	33	-0.04890	-0.20540	
0.00456			X	0.00001348	31	34	-0.02394	-0.17745	
0.00394			Y	-0.00005175	31	35	0.08135	0.24394	-
0.00542			Z	0.05102848	31	36	-0.00004	-0.00009	
0.00000		10	S	0.00000865	31	37	-0.00061	0.00000	
0.00000			X	0.00002630	31	38	-0.00093	0.00000	
0.00000			Y	-0.00000007	31	39	0.00115	0.00000	
0.00000			Z	-0.18530971	31	40	0.00000	0.00000	
0.00000		11	S	0.00000823	31	41	-0.00001	-0.00046	
0.00001			X	-0.00000757	31	42	0.00231	0.00064	-
0.00001			Y	0.00000029	31	43	-0.00237	0.00035	-
0.00001			Z	0.10907555	31	44	0.00000	0.00000	
0.00000		12	S	-0.00003324	31	45	0.03361	-0.03357	
0.00107			X	0.00007586	31	46	-0.00518	0.05634	-
0.00180			Y	-0.00006697	31	47	0.01561	-0.18253	
0.00584			Z	0.01197287	31	48	0.00001	-0.00003	
0.00000		13	S	0.00000628	31	49	0.11482	-1.86732	
0.06552		14	S	-0.00001866	31	50	0.00030	-0.00001	
0.00000		15	S	-0.00000700	31	51	0.00442	-0.00231	
0.00008		16	S	0.00000297	31	52	0.00975	-0.00027	
0.00001		17	S	-0.00000967	31	53	0.00177	-0.00045	
0.00002		18	S	-0.00002046	31	54	-0.00172	-0.03232	
0.00113		19	S	-0.01336802	31	55	-0.00697	0.09422	-
0.00331		20	S	0.01343605	31	56	-0.00696	0.09421	-
0.00331									
32	AP	-9.767526	1	S	-0.00002784	32	1	-0.00002	0.00000
0.00000			X	0.00006187	32	2	0.00000	0.00000	
0.00000			Y	-0.00001970	32	3	0.00003	0.00000	
0.00000			Z	-0.47670689	32	4	0.00275	-0.00056	
0.00002		2	S	0.00000937	32	5	0.00005	0.00008	
0.00000			X	0.00003562	32	6	0.00006	0.00001	
0.00000			Y	0.00000028	32	7	-0.00004	-0.00013	
0.00000			Z	-0.47594237	32	8	-0.13578	-0.04019	
0.00129									

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00001	3	S	-0.00000146	32	9	-0.00002	0.00021	-
0.00001		X	0.00002095	32	10	-0.00004	-0.00016	
0.00001		Y	-0.00001464	32	11	0.00002	-0.00032	
0.00485		Z	-0.14056969	32	12	-0.08046	-0.15168	
0.00000	4	S	-0.00000257	32	13	-0.00003	0.00000	
0.00000		X	-0.00004565	32	14	0.00004	-0.00001	
0.00000		Y	0.00004041	32	15	0.00002	-0.00001	
0.00012		Z	0.39222723	32	16	-0.13555	-0.00360	
0.00000	5	S	-0.00003005	32	17	0.00001	0.00000	
0.00000		X	-0.00005064	32	18	0.00000	0.00000	
0.00000		Y	-0.00000427	32	19	-0.00002	0.00000	
0.00000		Z	0.55029857	32	20	0.02232	-0.00010	
0.00000	6	S	0.00001121	32	21	0.00000	0.00000	
0.00000		X	-0.00000897	32	22	-0.00001	0.00000	
0.00000		Y	-0.00000281	32	23	0.00000	0.00000	
0.00000		Z	0.05448740	32	24	0.09634	-0.00004	
0.00011	7	S	0.00000798	32	25	-0.00019	0.00356	-
0.00014		X	-0.00001729	32	26	0.00072	-0.00435	
0.00009		Y	0.00001550	32	27	0.00015	-0.00295	
0.08907		Z	-0.01142703	32	28	0.78928	-2.78345	
0.00000	8	S	-0.00000465	32	29	0.00018	0.00000	
0.00000		X	0.00005583	32	30	-0.00001	0.00000	
0.00000		Y	-0.00001473	32	31	0.00021	0.00000	
1.00000		Z	0.07233332	32	32	1.54932	0.00000	
0.00000	9	S	-0.00001331	32	33	0.00000	0.00007	
0.00000		X	-0.00002234	32	34	-0.00001	0.00006	
0.00000		Y	0.00003356	32	35	0.00001	-0.00009	
0.00054		Z	0.20424956	32	36	0.03425	-0.02425	
0.00000	10	S	0.00000018	32	37	0.00000	0.00000	
0.00000		X	0.00000443	32	38	0.00000	0.00000	
0.00000		Y	-0.00000248	32	39	0.00000	0.00000	
0.00000		Z	-0.02094535	32	40	-0.02295	0.00000	
0.00000	11	S	0.00000522	32	41	0.00000	0.00000	
0.00000		X	0.00001357	32	42	0.00000	0.00000	
0.00000		Y	-0.00002919	32	43	0.00000	0.00000	
0.00000		Z	-0.13888766	32	44	0.03030	-0.00005	
0.00002	12	S	-0.00002254	32	45	0.00003	0.00071	-
0.00004		X	-0.00000724	32	46	-0.00007	-0.00119	
0.00000		Y	-0.00004064	32	47	0.00003	-0.00003	
0.00589		Z	0.00266126	32	48	-0.08262	-0.18419	
0.00002	13	S	0.00003113	32	49	-0.00002	0.00046	-
0.00000	14	S	-0.00000005	32	50	0.00000	0.00000	
0.00000	15	S	0.00000727	32	51	0.00001	0.00000	
0.00000	16	S	0.00001493	32	52	-0.00001	0.00000	
0.00000	17	S	-0.00000422	32	53	-0.00001	0.00000	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000			18	S	-0.00000486	32	54	-0.00002	0.00008	
0.00531			19	S	-0.00261958	32	55	0.07990	0.15141	-
0.00529			20	S	0.00264244	32	56	-0.07991	-0.15083	
0.02432	33 AP	-2.347942	1	S	0.00003712	33	1	-0.01758	-0.76013	
0.02009				X	-0.00002571	33	2	0.00736	0.62767	-
0.03223				Y	-0.00001165	33	3	0.01276	1.00729	-
0.00000				Z	0.23692106	33	4	0.00001	0.00003	
0.22125			2	S	-0.00004334	33	5	0.20264	-6.91415	
0.26632				X	-0.00005089	33	6	-0.35222	8.32265	-
0.13863				Y	0.00002064	33	7	-0.18564	4.33227	-
0.00002				Z	0.31937373	33	8	-0.00004	0.00059	-
0.02074			3	S	-0.00000142	33	9	0.00613	-0.64808	
0.03252				X	0.00005428	33	10	0.00627	1.01640	-
0.00051				Y	-0.00001449	33	11	0.00452	-0.01585	
0.00000				Z	-0.41195348	33	12	0.00001	0.00010	
0.00067			4	S	0.00001279	33	13	0.01431	-0.02083	
0.00108				X	-0.00006914	33	14	-0.01422	0.03389	-
0.00019				Y	0.00001168	33	15	-0.00531	0.00608	-
0.00000				Z	0.42202532	33	16	-0.00001	0.00000	
0.00019			5	S	-0.00000465	33	17	0.00135	-0.00594	
0.00028				X	-0.00001780	33	18	-0.00167	0.00863	-
0.00016				Y	0.00001655	33	19	-0.00291	0.00487	-
0.00000				Z	0.09134983	33	20	-0.00001	0.00000	
0.00074			6	S	-0.00002279	33	21	0.02236	-0.02324	
0.00081				X	0.00004280	33	22	-0.01976	0.02540	-
0.00092				Y	-0.00001501	33	23	-0.01376	0.02877	-
0.00000				Z	-0.50462288	33	24	0.00000	0.00000	
0.00741			7	S	-0.00001096	33	25	-0.01021	-0.23168	
0.01026				X	-0.00024009	33	26	-0.00025	0.32049	-
0.00603				Y	0.00003839	33	27	-0.01151	-0.18844	
0.00000				Z	-0.36106050	33	28	0.00002	0.00003	
0.00370			8	S	0.00000655	33	29	-0.03778	-0.16636	
0.00302				X	0.00017257	33	30	0.05526	0.13591	-
0.00456				Y	-0.00000157	33	31	-0.04890	-0.20540	
0.00000				Z	0.26894552	33	32	0.00000	0.00007	
1.00000			9	S	0.00001906	33	33	1.65648	0.00000	
0.00000				X	0.00002544	33	34	-0.36150	0.00000	
0.00000				Y	-0.00004066	33	35	0.15352	0.00000	
0.00000				Z	-0.07052986	33	36	-0.00017	0.00000	
0.00000			10	S	-0.00000107	33	37	-0.00370	-0.00004	
0.00000				X	-0.00001787	33	38	0.00048	0.00003	
0.00000				Y	-0.00000768	33	39	0.00876	0.00005	
0.00000				Z	0.10097317	33	40	0.00000	0.00000	
0.00000			11	S	0.00000221	33	41	-0.00272	-0.00002	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000			X	0.00000579	33	42	0.00558	0.00004	
0.00000			Y	-0.00000743	33	43	-0.00288	0.00000	
0.00000			Z	-0.08142604	33	44	0.00000	0.00000	
0.00014		12	S	-0.00002273	33	45	-0.00218	-0.00445	
0.00021			X	0.00003091	33	46	0.00074	0.00648	-
0.00012			Y	-0.00002720	33	47	-0.00100	-0.00364	
0.00000			Z	0.03490780	33	48	0.00000	0.00000	
0.38420		13	S	-0.00002987	33	49	0.45358	-10.94972	
0.00001		14	S	0.00000959	33	50	0.00296	-0.00026	
0.01576		15	S	-0.00001994	33	51	-0.00625	-0.44916	
0.00003		16	S	0.00000742	33	52	0.00008	-0.00087	
0.00001		17	S	0.00000132	33	53	0.00225	-0.00017	
0.00010		18	S	-0.00000355	33	54	0.00186	-0.00291	
0.00009		19	S	-0.05172302	33	55	-0.00031	-0.00257	
0.00009		20	S	0.05175153	33	56	-0.00032	-0.00257	
0.01497	34 AP	-1.718466	1	S	0.00002298	34	1	-0.01878	-0.46788
0.00906			X	-0.00004701	34	2	0.00315	0.28322	-
0.02144			Y	0.00003022	34	3	0.03861	0.67013	-
0.00000			Z	0.41321075	34	4	0.00002	0.00002	
0.18559		2	S	-0.00000112	34	5	0.42666	-5.79981	
0.19019			X	0.00004865	34	6	-0.56849	5.94337	-
0.13142			Y	-0.00002581	34	7	-0.34611	4.10694	-
0.00002			Z	-0.53809679	34	8	-0.00007	0.00056	-
0.02431		3	S	0.00002070	34	9	-0.05657	-0.75963	
0.03755			X	0.00001137	34	10	0.05414	1.17332	-
0.00064			Y	0.00001573	34	11	-0.03482	-0.02004	
0.00000			Z	0.02312962	34	12	0.00003	0.00013	
0.00084		4	S	-0.00004040	34	13	0.04979	-0.02619	
0.00136			X	-0.00005071	34	14	-0.03485	0.04236	-
0.00026			Y	0.00002250	34	15	-0.02255	0.00803	-
0.00000			Z	0.48621553	34	16	-0.00001	0.00000	
0.00021		5	S	0.00005025	34	17	0.00155	-0.00671	
0.00031			X	0.00005148	34	18	-0.00238	0.00957	-
0.00018			Y	-0.00001164	34	19	0.00086	0.00575	-
0.00000			Z	-0.51908797	34	20	-0.00001	0.00000	
0.00063		6	S	-0.00002243	34	21	0.03324	-0.01962	
0.00063			X	-0.00001909	34	22	-0.02323	0.01983	-
0.00082			Y	0.00001434	34	23	-0.01714	0.02553	-
0.00000			Z	0.11041068	34	24	0.00001	0.00000	
0.00777		7	S	0.00000012	34	25	-0.01046	-0.24284	
0.01037			X	0.00002234	34	26	-0.00693	0.32391	-
0.00675			Y	-0.00001531	34	27	-0.00415	-0.21082	
0.00000			Z	0.02762543	34	28	0.00003	0.00003	
0.00302		8	S	-0.00000215	34	29	-0.01438	-0.13591	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00207		X	-0.00001289	34	30	0.02091	0.09316	-			
		Y	0.00000373	34	31	-0.02394	-0.17745				
0.00394		Z	-0.01936455	34	32	-0.00001	0.00006				
0.00000											
0.00000	9	S	-0.00000961	34	33	-0.36150	0.00000				
		X	-0.00001288	34	34	1.41553	0.00000				
1.00000		Y	0.00002748	34	35	-0.19106	0.00000				
0.00000		Z	0.10915296	34	36	-0.00008	0.00000				
0.00000	10	S	0.00000352	34	37	-0.00771	-0.00003				
		X	0.00000730	34	38	0.00012	0.00002				
0.00000		Y	-0.00000550	34	39	0.01780	0.00004				
0.00000		Z	-0.02074209	34	40	0.00000	0.00000				
0.00000	11	S	0.00000091	34	41	-0.01121	-0.00004				
		X	-0.00000498	34	42	0.02030	0.00006				
0.00000		Y	0.00000300	34	43	-0.01202	0.00000				
0.00000		Z	-0.08700474	34	44	0.00000	0.00000				
0.00000	12	S	0.00000288	34	45	-0.00143	-0.00505				
0.00016		X	0.00000106	34	46	-0.00330	0.00722	-			
0.00023		Y	0.00000403	34	47	-0.00265	-0.00431				
0.00014		Z	-0.00262184	34	48	0.00000	0.00000				
0.00000	13	S	0.00002408	34	49	0.12993	-1.24448				
0.04367	14	S	-0.00000358	34	50	0.00461	-0.00018				
0.00001	15	S	-0.00001718	34	51	-0.01858	-0.07579				
0.00266	16	S	-0.00002830	34	52	-0.00205	-0.00084				
0.00003	17	S	0.00000717	34	53	0.00811	-0.00018				
0.00001	18	S	0.00001204	34	54	-0.00126	-0.00308				
0.00011	19	S	0.00574110	34	55	0.00201	-0.00230				
0.00008	20	S	-0.00575327	34	56	0.00201	-0.00230				
0.00008											
	35	AP	-0.437801	1	S	-0.00001398	35	1	-0.03447	-0.75085	
0.02403		X	-0.00004874	35	2	-0.01222	0.67013	-			
0.02144		Y	0.00005121	35	3	0.02024	0.94107	-			
0.03011		Z	0.35863015	35	4	-0.00002	0.00004				
0.00000											
0.09661	2	S	0.00006458	35	5	0.21031	-3.01903				
		X	0.00005655	35	6	-0.30553	4.10694	-			
0.13142		Y	-0.00004364	35	7	-0.10367	0.19141	-			
0.00613		Z	-0.14663464	35	8	0.00003	0.00029	-			
0.00001											
0.00038	3	S	-0.00005200	35	9	0.01122	0.01185	-			
		X	0.00000313	35	10	0.00782	-0.02004				
0.00064		Y	0.00001829	35	11	0.00204	-0.11145				
0.00357		Z	-0.17745326	35	12	-0.00002	0.00000				
0.00000											
0.00015	4	S	-0.00001129	35	13	0.00791	-0.00470				
		X	0.00002198	35	14	-0.00614	0.00803	-			
0.00026		Y	0.00000589	35	15	-0.00047	-0.00096				
0.00003		Z	-0.08947709	35	16	0.00001	0.00000				
0.00000											
0.00012	5	S	-0.00000287	35	17	0.00097	-0.00379				



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00018		X	-0.00004141	35	18	0.00024	0.00575	-		
		Y	-0.00000335	35	19	-0.00345	0.00263	-		
0.00008		Z	0.30061433	35	20	0.00001	0.00000			
0.00000										
0.00071	6	S	-0.00000594	35	21	0.02612	-0.02222			
		X	0.00003334	35	22	-0.01959	0.02553	-		
0.00082		Y	-0.00001932	35	23	-0.01117	0.02621	-		
0.00084		Z	-0.43855914	35	24	-0.00002	0.00000			
0.00000										
0.00457	7	S	0.00005304	35	25	-0.00315	0.14278	-		
		X	0.00038549	35	26	0.00233	-0.21082			
0.00675		Y	-0.00002560	35	27	0.00112	0.08931	-		
0.00286		Z	0.62730461	35	28	-0.00007	-0.00002			
0.00000										
0.00456	8	S	-0.00000317	35	29	0.06587	0.20540	-		
		X	-0.00020613	35	30	-0.08897	-0.17745			
0.00394		Y	0.00001777	35	31	0.08135	0.24394	-		
0.00542		Z	-0.33715114	35	32	0.00001	-0.00009			
0.00000										
0.00000	9	S	-0.00001876	35	33	0.15352	0.00000			
		X	-0.00002498	35	34	-0.19106	0.00000			
0.00000		Y	0.00003299	35	35	1.29190	0.00000			
1.00000		Z	0.02629388	35	36	0.00024	0.00000			
0.00000										
0.00000	10	S	-0.00000425	35	37	-0.00517	-0.00005			
		X	-0.00001343	35	38	0.00003	0.00004			
0.00000		Y	-0.00000101	35	39	0.01066	0.00007			
0.00000		Z	0.07413426	35	40	0.00000	0.00000			
0.00000										
0.00000	11	S	-0.00000286	35	41	-0.00126	0.00000			
		X	-0.00000098	35	42	0.00531	0.00000			
0.00000		Y	0.00000148	35	43	-0.00360	0.00000			
0.00000		Z	0.01405049	35	44	0.00000	0.00000			
0.00000										
0.00000	12	S	-0.00002643	35	45	0.00462	0.00284	-		
0.00009		X	0.00000321	35	46	-0.00317	-0.00431			
0.00014		Y	-0.00001369	35	47	0.00006	0.00198	-		
0.00006		Z	-0.03780815	35	48	0.00001	0.00000			
0.00000										
0.32488	13	S	0.00002660	35	49	-0.82702	9.25903	-		
0.00001	14	S	0.00001134	35	50	0.00345	-0.00024			
0.01668	15	S	0.00000303	35	51	0.00647	-0.47552			
0.00002										
	16	S	0.00000680	35	52	-0.00102	-0.00048			
0.00000	17	S	0.00000290	35	53	0.00021	-0.00002			
0.00003	18	S	0.00001011	35	54	-0.00523	0.00097	-		
0.00006	19	S	0.07965270	35	55	0.00052	0.00161	-		
0.00006	20	S	-0.07964247	35	56	0.00053	0.00161	-		
	36	AP	0.528821	1	S	0.00007917	36	1	-0.00002	-0.00003
0.00000										
		X	-0.00003574	36	2	0.00002	0.00002			
0.00000		Y	-0.00001502	36	3	0.00000	0.00004			
0.00000		Z	0.32542425	36	4	-0.11819	-0.13435			
0.00430										
0.00001	2	S	-0.00009434	36	5	0.00003	-0.00041			

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00002		X	-0.00000481	36	6	-0.00007	0.00056	-
		Y	-0.00000108	36	7	-0.00002	0.00029	-
0.00001		Z	-0.39698735	36	8	0.22213	-1.94641	
0.06229	3	S	0.00010078	36	9	-0.00001	-0.00007	
0.00000		X	-0.00005881	36	10	0.00002	0.00013	
0.00000		Y	-0.00001417	36	11	-0.00001	0.00000	
0.00000		Z	0.46634698	36	12	-0.11480	-0.11176	
0.00358	4	S	0.00000307	36	13	0.00001	0.00000	
0.00000		X	0.00005095	36	14	-0.00001	0.00000	
0.00000		Y	-0.00000409	36	15	0.00000	0.00000	
0.00000		Z	-0.33861524	36	16	0.00236	-0.00240	
0.00008	5	S	-0.00001464	36	17	-0.00001	0.00000	
0.00000		X	-0.00004295	36	18	-0.00001	0.00000	
0.00000		Y	0.00001225	36	19	0.00000	0.00000	
0.00000		Z	0.28327838	36	20	0.07336	-0.00061	
0.00002	6	S	-0.00002808	36	21	0.00001	0.00000	
0.00000		X	0.00005137	36	22	0.00000	0.00000	
0.00000		Y	-0.00000734	36	23	-0.00001	0.00000	
0.00000		Z	-0.29662207	36	24	-0.03344	-0.00271	
0.00009	7	S	-0.00008129	36	25	-0.00001	-0.00002	
0.00000		X	-0.00026235	36	26	-0.00003	0.00003	
0.00000		Y	-0.00001360	36	27	0.00000	-0.00002	
0.00000		Z	-0.42776152	36	28	-0.03402	-0.03464	
0.00111	8	S	-0.00000006	36	29	-0.00003	-0.00007	
0.00000		X	0.00012110	36	30	0.00007	0.00006	
0.00000		Y	-0.00001139	36	31	-0.00004	-0.00009	
0.00000		Z	0.19612245	36	32	0.03425	-0.02425	
0.00054	9	S	0.00000965	36	33	-0.00017	0.00000	
0.00000		X	0.00001885	36	34	-0.00008	0.00000	
0.00000		Y	0.00000926	36	35	0.00024	0.00000	
0.00000		Z	0.06536946	36	36	1.95629	0.00000	
1.00000	10	S	0.00000432	36	37	0.00000	0.00000	
0.00000		X	-0.00000996	36	38	0.00000	0.00000	
0.00000		Y	-0.00001166	36	39	0.00000	0.00000	
0.00000		Z	0.04543949	36	40	0.00893	0.00000	
0.00000	11	S	0.00000686	36	41	0.00000	0.00000	
0.00000		X	-0.00000198	36	42	0.00000	0.00000	
0.00000		Y	0.00000435	36	43	0.00000	0.00000	
0.00000		Z	0.05015751	36	44	0.00021	0.00000	
0.00000	12	S	0.00005989	36	45	-0.00001	0.00000	
0.00000		X	-0.00003859	36	46	0.00001	0.00000	
0.00000		Y	0.00003328	36	47	-0.00001	0.00000	
0.00000		Z	0.01796365	36	48	0.00513	-0.00045	
0.00001	13	S	0.00000189	36	49	0.00039	-0.00438	
0.00015	14	S	0.00000186	36	50	0.00000	0.00000	
0.00000								

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		15	S	-0.00004656	36	51	0.00000	0.00002	
0.00000		16	S	0.00000974	36	52	0.00000	0.00000	
0.00000		17	S	-0.00001370	36	53	0.00000	0.00000	
0.00000		18	S	-0.00001545	36	54	0.00000	0.00000	
0.00002		19	S	-0.05250165	36	55	-0.00588	0.00050	-
0.00002		20	S	0.05246146	36	56	0.00589	-0.00049	
0.02230	37 A* 1.078832	1	S	-0.27582273	37	1	-0.01762	-0.69698	
0.01678			X	-0.07789988	37	2	-0.01050	-0.52451	
0.03061			Y	0.06722728	37	3	-0.01775	-0.95665	
0.00000			Z	0.00005732	37	4	0.00001	0.00000	
0.00069		2	S	0.34518951	37	5	0.02165	-0.02161	
0.00037			X	0.10756046	37	6	0.00288	-0.01144	
0.00108			Y	-0.01342443	37	7	0.02554	-0.03382	
0.00000			Z	-0.00004323	37	8	0.00000	0.00000	
0.00017		3	S	-0.46014372	37	9	-0.00005	-0.00519	
0.00000			X	-0.02996498	37	10	0.00047	0.00005	
0.00028			Y	-0.06587067	37	11	0.00146	-0.00866	
0.00000			Z	0.00010395	37	12	0.00000	0.00000	
0.00068		4	S	0.39999419	37	13	0.01563	-0.02135	
0.00037			X	-0.07891443	37	14	-0.00313	0.01168	-
0.00107			Y	-0.01081575	37	15	0.01920	-0.03329	
0.00000			Z	-0.00000419	37	16	0.00000	0.00000	
0.02242		5	S	-0.31563672	37	17	-0.00090	-0.70052	
0.01710			X	0.06682255	37	18	-0.00783	0.53447	-
0.03063			Y	0.08526824	37	19	-0.01220	-0.95729	
0.00000			Z	-0.00002406	37	20	0.00000	0.00007	
0.22271		6	S	0.27494428	37	21	0.20869	-6.95954	
0.00092			X	0.01797690	37	22	-0.00293	0.02877	-
0.30194			Y	-0.05752056	37	23	0.40391	-9.43570	
0.00002			Z	-0.00002956	37	24	-0.00003	0.00048	-
0.00000		7	S	0.20295724	37	25	0.00145	-0.00007	
0.00000			X	0.01411165	37	26	-0.00001	0.00000	
0.00000			Y	0.15960443	37	27	0.00090	-0.00012	
0.00000			Z	-0.00011581	37	28	0.00000	0.00000	
0.00000		8	S	-0.01875859	37	29	-0.00036	0.00000	
0.00000			X	-0.03121197	37	30	0.00031	0.00000	
0.00000			Y	-0.06463024	37	31	-0.00061	0.00000	
0.00000			Z	0.00006604	37	32	0.00000	0.00000	
0.00000		9	S	-0.05781429	37	33	-0.00370	-0.00004	
0.00000			X	-0.13601008	37	34	-0.00771	-0.00003	
0.00000			Y	-0.05023300	37	35	-0.00517	-0.00005	
0.00000			Z	-0.00000570	37	36	0.00000	0.00000	
1.00000		10	S	-0.05778390	37	37	1.64778	0.00000	
0.00000			X	-0.02199536	37	38	-0.32430	0.00000	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000			Y	0.11895385	37	39	0.23486	0.00000		
0.00000			Z	-0.00000721	37	40	-0.00011	0.00000		
0.00000		11	S	-0.09510632	37	41	-0.00122	-0.00004		
0.00000			X	0.11593518	37	42	0.00536	0.00003		
0.00000			Y	-0.10725107	37	43	-0.00448	-0.00005		
0.00000			Z	0.00003035	37	44	0.00000	0.00000		
0.00000		12	S	-0.08643271	37	45	-0.00043	-0.00001		
0.00000			X	0.06379706	37	46	0.00053	0.00000		
0.00000			Y	-0.04836424	37	47	-0.00035	-0.00001		
0.00000			Z	-0.00004038	37	48	0.00000	0.00000		
0.00001		13	S	0.01068983	37	49	0.00316	-0.00025		
0.38752		14	S	0.01986062	37	50	0.45846	-11.04438		
0.01388		15	S	0.13114764	37	51	-0.00607	-0.39553		
0.01416		16	S	0.14658508	37	52	-0.01632	-0.40362		
0.00007		17	S	0.06559355	37	53	-0.00086	-0.00210		
0.00000		18	S	0.01551890	37	54	0.00043	-0.00013		
0.00000		19	S	0.03329481	37	55	0.00005	-0.00001		
0.00000		20	S	0.03331475	37	56	0.00005	-0.00001		
0.01253	38 A*	2.278873	1	S	-0.28653792	38	1	0.01790	0.39154	-
0.00629			X	-0.14717817	38	2	0.00491	0.19658	-	
0.01857			Y	-0.13746029	38	3	-0.00892	0.58022	-	
0.00000			Z	0.00001692	38	4	0.00002	0.00000		
0.00028		2	S	-0.08019330	38	5	-0.00487	0.00884	-	
0.00008			X	-0.12805204	38	6	0.00123	0.00242	-	
0.00047			Y	0.20830137	38	7	-0.00413	0.01455	-	
0.00000			Z	-0.00000501	38	8	0.00001	0.00000		
0.00000		3	S	0.38596156	38	9	-0.00243	-0.00004		
0.00002			X	0.00628966	38	10	-0.00491	-0.00053		
0.00000			Y	-0.08710822	38	11	-0.00175	-0.00007		
0.00000			Z	-0.00006153	38	12	-0.00001	0.00000		
0.00029		4	S	-0.07198322	38	13	0.01936	-0.00903		
0.00009			X	0.11247803	38	14	0.00139	0.00272	-	
0.00047			Y	0.23612952	38	15	0.02092	-0.01479		
0.00000			Z	0.00001976	38	16	0.00000	0.00000		
0.01277		5	S	-0.32018632	38	17	-0.04615	-0.39895		
0.00660			X	0.13938650	38	18	0.01024	0.20638	-	
0.01884			Y	-0.13138759	38	19	-0.01119	-0.58863		
0.00000			Z	-0.00002255	38	20	0.00002	0.00004		
0.00064		6	S	0.45292854	38	21	0.01059	-0.02004		
0.06281			X	0.01534826	38	22	0.06419	-1.96291		
0.00098			Y	-0.05712692	38	23	0.02818	-0.03072		
0.00000			Z	-0.00001668	38	24	-0.00003	0.00000		
0.00000		7	S	-0.26246870	38	25	0.00132	0.00000		
0.00000			X	-0.04365547	38	26	0.00032	-0.00001		

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000			Y	-0.14097813	38	27	0.00128	0.00000			
0.00000			Z	0.00008348	38	28	0.00000	0.00000			
0.00000		8	S	0.02237725	38	29	-0.00022	0.00000			
0.00000			X	0.05505653	38	30	-0.00057	0.00000			
0.00000			Y	0.05919059	38	31	-0.00093	0.00000			
0.00000			Z	-0.00004749	38	32	0.00000	0.00000			
0.00000		9	S	-0.00384204	38	33	0.00048	0.00003			
0.00000			X	0.02983273	38	34	0.00012	0.00002			
0.00000			Y	-0.00138465	38	35	0.00003	0.00004			
0.00000			Z	-0.00000834	38	36	0.00000	0.00000			
0.00000		10	S	-0.08760312	38	37	-0.32430	0.00000			
0.00000			X	-0.02306570	38	38	1.42649	0.00000			
1.00000			Y	0.18110758	38	39	-0.17713	0.00000			
0.00000			Z	-0.00001322	38	40	-0.00016	0.00000			
0.00000		11	S	0.03324829	38	41	-0.00172	-0.00003			
0.00000			X	-0.00967632	38	42	0.00465	0.00002			
0.00000			Y	-0.00029789	38	43	-0.00407	-0.00005			
0.00000			Z	-0.00001736	38	44	0.00000	0.00000			
0.00000		12	S	0.15194368	38	45	0.00018	0.00000			
0.00000			X	-0.09960611	38	46	-0.00009	0.00000			
0.00000			Y	0.05421846	38	47	0.00016	0.00000			
0.00000			Z	0.00006697	38	48	0.00000	0.00000			
0.00000		13	S	0.02760692	38	49	-0.00054	0.00011			
0.00000		14	S	0.02449751	38	50	0.82015	-8.82232			
0.30956		15	S	0.13432318	38	51	-0.01228	0.33082	-		
0.01161		16	S	0.15850629	38	52	-0.00437	-0.33991			
0.01193		17	S	-0.05605970	38	53	-0.00089	-0.00162			
0.00006		18	S	-0.03725455	38	54	0.00056	-0.00005			
0.00000		19	S	-0.06023836	38	55	-0.00017	0.00000			
0.00000		20	S	-0.06024493	38	56	-0.00017	0.00000			
0.00000											
0.02285	39	A*	2.576759	1	S	-0.43676797	39	1	0.03136	0.71413	-
0.01857					X	0.00418356	39	2	0.04029	0.58022	-
0.02997					Y	0.12738019	39	3	0.02661	0.93672	-
0.00000					Z	0.00004699	39	4	0.00000	0.00000	
0.00084				2	S	0.36491978	39	5	-0.03979	0.02613	-
0.00047					X	-0.01780160	39	6	-0.00432	0.01455	-
0.00130					Y	0.15920182	39	7	-0.03891	0.04048	-
0.00000					Z	-0.00001144	39	8	0.00000	0.00000	
0.00022				3	S	-0.01471817	39	9	-0.00036	0.00674	-
0.00000					X	0.28877658	39	10	0.00119	-0.00007	
0.00036					Y	0.01173410	39	11	-0.00072	0.01122	-
0.00000					Z	0.00005876	39	12	0.00000	0.00000	
0.00082				4	S	-0.35033816	39	13	-0.04281	0.02572	-
0.00047					X	-0.04098870	39	14	0.00338	-0.01479	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00127		Y	-0.13918164	39	15	-0.04166	0.03968	-
0.00000		Z	-0.00004051	39	16	0.00000	0.00000	
0.02287	5	S	0.37775832	39	17	0.03894	0.71455	-
0.01884		X	0.04465366	39	18	-0.04920	-0.58863	
0.02983		Y	-0.13880138	39	19	0.02661	0.93205	-
0.00000		Z	0.00006451	39	20	0.00000	-0.00008	
0.21034	6	S	0.04308168	39	21	-0.46957	6.57301	-
0.00098		X	-0.29828224	39	22	-0.00011	-0.03072	
0.25953		Y	-0.00175351	39	23	-0.72928	8.11025	-
0.00002		Z	-0.00004460	39	24	0.00004	-0.00051	
0.00000	7	S	0.02643730	39	25	-0.00100	0.00010	
0.00000		X	0.00395049	39	26	-0.00044	0.00000	
0.00001		Y	0.00481681	39	27	0.00059	0.00017	-
0.00000		Z	-0.00009881	39	28	0.00000	0.00000	
0.00000	8	S	0.00092022	39	29	0.00076	0.00000	
0.00000		X	0.00847160	39	30	-0.00051	0.00000	
0.00000		Y	0.00638790	39	31	0.00115	0.00000	
0.00000		Z	0.00003438	39	32	0.00000	0.00000	
0.00000	9	S	-0.06653934	39	33	0.00876	0.00005	
0.00000		X	-0.11838914	39	34	0.01780	0.00004	
0.00000		Y	-0.06139908	39	35	0.01066	0.00007	
0.00000		Z	-0.00001647	39	36	0.00000	0.00000	
0.00000	10	S	-0.02141036	39	37	0.23486	0.00000	
0.00000		X	0.01862511	39	38	-0.17713	0.00000	
1.00000		Y	0.01359016	39	39	1.26120	0.00000	
0.00000		Z	-0.00000133	39	40	-0.00002	0.00000	
0.00000	11	S	0.07481371	39	41	0.00725	0.00005	
0.00000		X	-0.09658103	39	42	-0.01704	-0.00005	
0.00000		Y	0.09988435	39	43	0.01595	0.00007	
0.00000		Z	-0.00001589	39	44	0.00000	0.00000	
0.00000	12	S	-0.04788065	39	45	0.00090	0.00001	
0.00000		X	0.03123363	39	46	-0.00005	0.00000	
0.00000		Y	-0.00734916	39	47	0.00086	0.00001	
0.00000		Z	-0.00002261	39	48	0.00000	0.00000	
0.00001	13	S	0.02949764	39	49	-0.00589	0.00026	-
0.11413	14	S	0.03479687	39	50	0.27714	-3.25283	
0.00936	15	S	0.23009038	39	51	0.01393	0.26681	-
0.00944	16	S	-0.20478143	39	52	0.00944	0.26912	-
0.00006	17	S	-0.03659221	39	53	0.00105	0.00167	-
0.00000	18	S	0.00450596	39	54	-0.00118	0.00014	
0.00000	19	S	0.02487610	39	55	0.00006	0.00001	
0.00000	20	S	0.02490276	39	56	0.00006	0.00001	
0.00000	40	A*	3.466581	1	S	-0.02482556	0.00000	
0.00000		X	-0.04488453	40	2	0.00001	0.00000	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		Y	-0.11598112	40	3	-0.00001	0.00000
		Z	0.00000787	40	4	-0.11345	-0.12154
0.00389	2	S	-0.19282073	40	5	0.00001	0.00000
0.00000		X	-0.01750878	40	6	0.00000	0.00000
0.00000		Y	0.04624214	40	7	0.00000	0.00000
0.00000		Z	-0.00002073	40	8	-0.02900	-0.00250
0.00008	3	S	0.08638154	40	9	0.00000	0.00000
0.00000		X	-0.01497670	40	10	-0.00001	0.00000
0.00000		Y	0.30893755	40	11	0.00000	0.00000
0.00000		Z	0.00002941	40	12	0.06808	-0.00053
0.00002	4	S	-0.17814068	40	13	0.00000	0.00000
0.00000		X	0.01713727	40	14	0.00000	0.00000
0.00000		Y	0.08853248	40	15	0.00000	0.00000
0.00000		Z	-0.00002591	40	16	-0.02102	-0.00247
0.00008	5	S	-0.09867343	40	17	0.00000	-0.00005
0.00000		X	0.03204874	40	18	0.00001	0.00004
0.00000		Y	-0.12615591	40	19	-0.00001	-0.00008
0.00000		Z	0.00000075	40	20	-0.11030	-0.12226
0.00391	6	S	0.13076884	40	21	0.00003	-0.00033
0.00001		X	0.03410835	40	22	-0.00001	0.00000
0.00000		Y	-0.01104762	40	23	0.00005	-0.00051
0.00002		Z	-0.00000382	40	24	0.19847	-1.96301
0.06282	7	S	0.35912117	40	25	0.00000	0.00000
0.00000		X	0.21402484	40	26	0.00002	0.00000
0.00000		Y	-0.07800906	40	27	0.00000	0.00000
0.00000		Z	-0.00018099	40	28	0.01993	-0.00001
0.00000	8	S	-0.03791111	40	29	0.00000	0.00000
0.00000		X	-0.10588643	40	30	-0.00002	0.00000
0.00000		Y	-0.03273983	40	31	0.00000	0.00000
0.00000		Z	0.00006893	40	32	-0.02295	0.00000
0.00000	9	S	0.04791469	40	33	0.00000	0.00000
0.00000		X	0.10548250	40	34	0.00000	0.00000
0.00000		Y	0.03832160	40	35	0.00000	0.00000
0.00000		Z	0.00001196	40	36	0.00893	0.00000
0.00000	10	S	-0.01954686	40	37	-0.00011	0.00000
0.00000		X	-0.00406166	40	38	-0.00016	0.00000
0.00000		Y	0.04449744	40	39	-0.00002	0.00000
0.00000		Z	-0.00000215	40	40	1.96363	0.00000
1.00000	11	S	-0.00007196	40	41	0.00000	0.00000
0.00000		X	-0.11721320	40	42	0.00000	0.00000
0.00000		Y	0.06150284	40	43	0.00000	0.00000
0.00000		Z	0.00005472	40	44	0.00619	0.00000
0.00000	12	S	-0.54940593	40	45	0.00000	0.00000
0.00000		X	0.16117465	40	46	0.00000	0.00000
0.00000		Y	-0.06627731	40	47	0.00000	0.00000

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		Z	-0.00013534	40	48	-0.00323	0.00000	
0.00000		13	S	-0.00216313	40	49	0.00000	0.00000
0.00009		14	S	0.00018026	40	50	0.00023	-0.00247
0.00000		15	S	0.03930942	40	51	0.00000	0.00003
0.00000		16	S	0.09268644	40	52	-0.00001	-0.00005
0.00000		17	S	0.05213116	40	53	0.00000	0.00000
0.00000		18	S	0.25743961	40	54	0.00000	0.00000
0.00000		19	S	0.24029909	40	55	0.00361	0.00000
0.00000		20	S	0.24034844	40	56	-0.00362	0.00000
0.00000								
0.00018	41 A*	1	S	-0.00649010	41	1	0.00151	-0.00571
0.00027		X	-0.00959436	41	2	0.00177	-0.00838	
0.00015		Y	0.04741132	41	3	-0.00188	0.00454	-
0.00000		Z	-0.00000514	41	4	0.00000	0.00000	
0.00064		2	S	0.07257199	41	5	0.01930	-0.02013
0.00105		X	-0.04105598	41	6	0.02061	-0.03285	
0.00017		Y	0.02401260	41	7	-0.00876	0.00536	-
0.00000		Z	-0.00000013	41	8	0.00000	0.00000	
0.01989		3	S	0.11998581	41	9	-0.01037	-0.62154
0.03121		X	-0.06860259	41	10	-0.02735	-0.97542	
0.00108		Y	-0.28741223	41	11	-0.00483	-0.03362	
0.00000		Z	-0.00001167	41	12	0.00000	-0.00010	
0.22014		4	S	0.14753591	41	13	0.21233	-6.87946
0.26928		X	0.15407749	41	14	0.37052	-8.41502	
0.12984		Y	-0.09591022	41	15	-0.18223	4.05735	-
0.00004		Z	0.00003929	41	16	0.00006	-0.00137	
0.02463		5	S	0.11011903	41	17	-0.00389	-0.76962
0.02113		X	0.04087856	41	18	-0.01397	-0.66031	
0.03211		Y	0.08921382	41	19	-0.00063	1.00346	-
0.00000		Z	0.00001336	41	20	-0.00001	-0.00014	
0.00074		6	S	-0.01680132	41	21	0.01683	-0.02316
0.00083		X	-0.04531866	41	22	0.01595	-0.02586	
0.00090		Y	0.01718681	41	23	-0.01191	0.02817	-
0.00000		Z	-0.00000380	41	24	0.00000	0.00000	
0.00680		7	S	-0.26212484	41	25	-0.00616	-0.21252
0.00935		X	0.02241681	41	26	0.00234	-0.29229	
0.00566		Y	-0.17204660	41	27	-0.00418	-0.17673	
0.00000		Z	0.00000217	41	28	0.00000	-0.00004	
0.00001		8	S	0.02786349	41	29	-0.00187	-0.00055
0.00002		X	0.05297136	41	30	-0.00492	-0.00074	
0.00001		Y	0.06844875	41	31	-0.00001	-0.00046	
0.00000		Z	-0.00002756	41	32	0.00000	0.00000	
0.00000		9	S	-0.03545105	41	33	-0.00272	-0.00002
0.00000		X	-0.05932052	41	34	-0.01121	-0.00004	
0.00000		Y	-0.01593950	41	35	-0.00126	0.00000	



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		Z	-0.00001215	41	36	0.00000	0.00000			
0.00000		10	S	-0.00719929	41	37	-0.00122	-0.00004		
0.00000		X	0.00074958	41	38	-0.00172	-0.00003			
0.00000		Y	0.01049800	41	39	0.00725	0.00005			
0.00000		Z	-0.00000118	41	40	0.00000	0.00000			
1.00000		11	S	-0.28688264	41	41	1.66198	0.00000		
0.00000		X	-0.08931936	41	42	0.07303	0.00000			
0.00000		Y	-0.26794076	41	43	-0.35523	0.00000			
0.00000		Z	0.00010232	41	44	0.00008	0.00000			
0.02077		12	S	-0.25965628	41	45	-0.07476	-0.64899		
0.01622		X	-0.28449914	41	46	-0.08521	-0.50696			
0.02825		Y	0.02832931	41	47	-0.07489	-0.88268			
0.00002		Z	0.00019137	41	48	0.00007	-0.00048			
0.00005		13	S	0.01858362	41	49	0.00015	-0.00157		
0.00009		14	S	0.00592149	41	50	-0.00077	-0.00246		
0.00003		15	S	-0.03891923	41	51	0.00049	-0.00084		
0.01626		16	S	-0.16934903	41	52	-0.01669	-0.46333		
0.33799		17	S	0.47992361	41	53	0.42924	-9.63264		
0.14724		18	S	0.26679263	41	54	0.09151	-4.19636		
0.00501		19	S	0.16386883	41	55	0.01395	-0.14278		
0.00502		20	S	0.16385205	41	56	0.01391	-0.14312		
0.00021	42 A*	4.867642	1	S	-0.07050632	42	1	-0.00297	0.00652	-
0.00030		X	-0.11169558	42	2	-0.00283	0.00940		-	
0.00017		Y	-0.27420411	42	3	0.00049	-0.00541			
0.00000		Z	0.00000467	42	4	0.00000	0.00000			
0.00081		2	S	-0.28429303	42	5	-0.03718	0.02540		-
0.00132		X	0.02440933	42	6	-0.03075	0.04122			-
0.00023		Y	0.05503087	42	7	0.01533	-0.00710			
0.00000		Z	-0.00000878	42	8	-0.00001	0.00000			
0.02334		3	S	-0.05653258	42	9	0.03381	0.72948		-
0.03609		X	-0.27799317	42	10	0.04010	1.12778			-
0.00136		Y	0.20474410	42	11	0.02170	0.04254			-
0.00000		Z	-0.00002889	42	12	0.00000	0.00013			
0.18771		4	S	0.09252586	42	13	-0.40171	5.86584		-
0.19757		X	0.00661193	42	14	-0.54710	6.17399			-
0.12509		Y	-0.20943609	42	15	0.31098	-3.90919			
0.00004		Z	0.00001005	42	16	-0.00011	0.00132			-
0.01575		5	S	0.23079680	42	17	0.01423	0.49210		-
0.01024		X	0.28978860	42	18	-0.00599	0.32011			-
0.02220		Y	0.07619699	42	19	-0.04185	-0.69359			
0.00000		Z	0.00005488	42	20	0.00001	0.00010			
0.00064		6	S	0.21726654	42	21	-0.02908	0.01997		-
0.00066		X	-0.16104786	42	22	-0.02076	0.02075			-
0.00082		Y	0.07374147	42	23	0.01530	-0.02554			

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		Z	-0.00002680	42	24	0.00000	0.00000	
0.00709		7 S	0.15310054	42	25	0.01394	0.22168	-
0.00940		X	-0.01079958	42	26	0.00131	0.29374	-
0.00629		Y	0.10510371	42	27	0.00415	0.19662	-
0.00000		Z	0.00000978	42	28	0.00000	0.00004	
0.00002		8 S	-0.02132622	42	29	-0.00211	0.00074	-
0.00002		X	-0.04124296	42	30	-0.00598	0.00098	-
0.00001		Y	-0.04566351	42	31	0.00231	0.00064	-
0.00000		Z	0.00001896	42	32	0.00000	0.00000	
0.00000		9 S	0.07099868	42	33	0.00558	0.00004	
0.00000		X	0.13948706	42	34	0.02030	0.00006	
0.00000		Y	0.05734177	42	35	0.00531	0.00000	
0.00000		Z	0.00001448	42	36	0.00000	0.00000	
0.00000		10 S	-0.07685683	42	37	0.00536	0.00003	
0.00000		X	-0.01052785	42	38	0.00465	0.00002	
0.00000		Y	0.13367303	42	39	-0.01704	-0.00005	
0.00000		Z	-0.00001119	42	40	0.00000	0.00000	
0.00000		11 S	-0.10212966	42	41	0.07303	0.00000	
0.00000		X	-0.01321588	42	42	1.14306	0.00000	
1.00000		Y	-0.14021766	42	43	-0.05713	0.00000	
0.00000		Z	0.00000086	42	44	-0.00007	0.00000	
0.00000		12 S	0.17313191	42	45	-0.00113	0.37888	-
0.01212		X	0.08345251	42	46	-0.00701	0.20731	-
0.00663		Y	-0.16227719	42	47	-0.01609	0.55587	-
0.01779		Z	0.00002045	42	48	-0.00001	0.00030	-
0.00001		13 S	-0.00937602	42	49	0.00076	0.00170	-
0.00006		14 S	0.03168317	42	50	0.00046	0.00090	-
0.00003		15 S	0.06086126	42	51	0.00212	0.00082	-
0.00003		16 S	-0.37568942	42	52	0.00622	0.08923	-
0.00313		17 S	0.18224354	42	53	0.63344	-6.58164	
0.23093		18 S	-0.07060547	42	54	-0.03963	1.31518	-
0.04615		19 S	-0.17057295	42	55	-0.00035	0.05789	-
0.00203		20 S	-0.17069916	42	56	-0.00035	0.05799	-
0.00203								
0.00011	43 A*	5.017333	1 S	0.23547973	43	1	-0.00174	-0.00353
0.00017			X	-0.34981063	43	2	-0.00321	-0.00541
0.00008			Y	0.08760366	43	3	-0.00354	0.00234
0.00000			Z	-0.00007095	43	4	0.00000	0.00000
0.00013			2 S	0.11221411	43	5	0.01810	-0.00414
0.00023			X	0.01408168	43	6	0.01638	-0.00710
0.00004			Y	-0.16856048	43	7	-0.00591	-0.00116
0.00000			Z	0.00001104	43	8	0.00001	0.00000
0.00080			3 S	-0.02691618	43	9	-0.00321	0.02514
0.00136			X	0.10589542	43	10	-0.02615	0.04254
0.00336			Y	-0.09367865	43	11	-0.00787	-0.10504

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00000		Z	0.00001543	43	12	-0.00001	0.00000	
0.09050	4	S	-0.01438717	43	13	0.22050	-2.82824	
0.12509		X	-0.04725978	43	14	0.34668	-3.90919	
0.00157		Y	-0.02708877	43	15	-0.11494	-0.04891	
0.00002		Z	-0.00000023	43	16	0.00006	-0.00064	
0.02393	5	S	0.08534001	43	17	-0.05474	-0.74784	
0.02220		X	0.32262084	43	18	-0.00154	-0.69359	
0.02937		Y	-0.00947564	43	19	0.02746	0.91775	-
0.00000		Z	0.00004385	43	20	-0.00001	-0.00015	
0.00070	6	S	0.26009008	43	21	0.03824	-0.02176	
0.00082		X	0.08582307	43	22	0.03271	-0.02554	
0.00080		Y	0.13513932	43	23	-0.01754	0.02513	-
0.00000		Z	-0.00000684	43	24	0.00000	0.00000	
0.00429	7	S	-0.05225644	43	25	-0.01019	0.13404	-
0.00629		X	0.02262490	43	26	-0.00399	0.19662	-
0.00280		Y	-0.06679866	43	27	-0.00606	0.08745	-
0.00000		Z	-0.00000902	43	28	-0.00001	0.00002	
0.00001	8	S	0.00724325	43	29	0.00131	0.00046	-
0.00001		X	0.01711903	43	30	0.00481	0.00064	-
0.00001		Y	0.01654629	43	31	-0.00237	0.00035	-
0.00000		Z	-0.00000867	43	32	0.00000	0.00000	
0.00000	9	S	-0.05415900	43	33	-0.00288	0.00000	
0.00000		X	-0.10711086	43	34	-0.01202	0.00000	
0.00000		Y	-0.03384833	43	35	-0.00360	0.00000	
0.00000		Z	-0.00001282	43	36	0.00000	0.00000	
0.00000	10	S	-0.11092120	43	37	-0.00448	-0.00005	
0.00000		X	-0.03109290	43	38	-0.00407	-0.00005	
0.00000		Y	0.20424908	43	39	0.01595	0.00007	
0.00000		Z	-0.00001759	43	40	0.00000	0.00000	
0.00000	11	S	0.09549396	43	41	-0.35523	0.00000	
0.00000		X	0.14805645	43	42	-0.05713	0.00000	
0.00000		Y	0.13066375	43	43	1.52498	0.00000	
1.00000		Z	-0.00001036	43	44	0.00002	0.00000	
0.02111	12	S	-0.10865316	43	45	0.07128	0.65968	-
0.01779		X	0.02153578	43	46	0.05970	0.55587	-
0.02739		Y	0.14741530	43	47	0.04310	0.85589	-
0.00002		Z	-0.00008346	43	48	-0.00008	0.00053	-
0.00001	13	S	0.00964329	43	49	-0.00091	0.00037	-
0.00009	14	S	0.03126314	43	50	-0.00137	-0.00258	
0.00002	15	S	-0.44673344	43	51	0.00127	-0.00045	
0.01713	16	S	-0.28700426	43	52	-0.00880	-0.48833	
0.18646	17	S	-0.26299810	43	53	0.59877	-5.31399	
0.13653	18	S	-0.02309760	43	54	-0.18713	3.89121	-
0.00485	19	S	0.12442990	43	55	-0.00844	0.13823	-
0.00486	20	S	0.12454034	43	56	-0.00842	0.13861	-

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

44	A*	5.154883	1	S	0.16625819	44	1	0.00000	0.00000	
0.00000				X	-0.17301929	44	2	-0.00001	0.00000	
0.00000				Y	0.10072971	44	3	0.00000	0.00000	
0.00000				Z	-0.00004053	44	4	0.06776	-0.00059	
0.00002			2	S	0.11581665	44	5	-0.00001	0.00000	
0.00000				X	0.04008786	44	6	0.00000	0.00000	
0.00000				Y	-0.15169315	44	7	0.00000	0.00000	
0.00000				Z	0.00001433	44	8	0.00232	-0.00231	
0.00007			3	S	-0.06927533	44	9	0.00000	0.00008	
0.00000				X	0.26944089	44	10	0.00002	0.00013	
0.00000				Y	0.13825601	44	11	0.00000	0.00000	
0.00000				Z	0.00002215	44	12	-0.10483	-0.10651	
0.00341			4	S	-0.26806587	44	13	-0.00007	0.00096	-
0.00003				X	-0.00160484	44	14	-0.00013	0.00132	-
0.00004				Y	0.01117611	44	15	0.00005	-0.00064	
0.00002				Z	-0.00001940	44	16	0.18981	-1.93374	
0.06188			5	S	-0.08316945	44	17	0.00001	0.00010	
0.00000				X	-0.01623360	44	18	0.00001	0.00010	
0.00000				Y	-0.30566221	44	19	-0.00001	-0.00015	
0.00000				Z	-0.00000189	44	20	-0.11231	-0.13630	
0.00436			6	S	0.10771687	44	21	-0.00001	0.00000	
0.00000				X	0.15562722	44	22	-0.00001	0.00000	
0.00000				Y	0.03415942	44	23	0.00000	0.00000	
0.00000				Z	0.00000794	44	24	-0.02089	-0.00270	
0.00009			7	S	0.07232354	44	25	0.00000	0.00003	
0.00000				X	-0.06337056	44	26	-0.00003	0.00004	
0.00000				Y	0.13123885	44	27	0.00001	0.00002	
0.00000				Z	-0.00000173	44	28	-0.02893	-0.03144	
0.00101			8	S	-0.00898081	44	29	0.00001	0.00000	
0.00000				X	-0.01342778	44	30	0.00003	0.00000	
0.00000				Y	-0.02354512	44	31	0.00000	0.00000	
0.00000				Z	0.00001999	44	32	0.03030	-0.00005	
0.00000			9	S	-0.03081019	44	33	0.00000	0.00000	
0.00000				X	-0.06961624	44	34	0.00000	0.00000	
0.00000				Y	-0.02810014	44	35	0.00000	0.00000	
0.00000				Z	-0.00000429	44	36	0.00021	0.00000	
0.00000			10	S	-0.02532702	44	37	0.00000	0.00000	
0.00000				X	-0.00263412	44	38	0.00000	0.00000	
0.00000				Y	0.06503764	44	39	0.00000	0.00000	
0.00000				Z	-0.00000214	44	40	0.00619	0.00000	
0.00000			11	S	-0.08779027	44	41	0.00008	0.00000	
0.00000				X	-0.32747221	44	42	-0.00007	0.00000	
0.00000				Y	-0.14124879	44	43	0.00002	0.00000	
0.00000				Z	0.00000280	44	44	1.96617	0.00000	
1.00000										

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00001		12	S	0.16477107	44	45	0.00012	0.00036	-
0.00001			X	-0.06162859	44	46	0.00014	0.00030	-
0.00002			Y	-0.24370104	44	47	0.00012	0.00053	-
0.00358			Z	0.00016323	44	48	0.00665	-0.11195	
0.00000		13	S	-0.00577417	44	49	0.00000	0.00000	
0.00000		14	S	-0.01062747	44	50	0.00000	0.00000	
0.00000		15	S	-0.25492683	44	51	0.00000	0.00000	
0.00000		16	S	0.16422209	44	52	0.00000	0.00003	
0.00001		17	S	0.39464790	44	53	-0.00003	0.00032	-
0.00016		18	S	0.05463424	44	54	-0.00024	0.00449	-
0.00146		19	S	-0.19138485	44	55	-0.00285	0.04174	-
0.00146		20	S	-0.19157203	44	56	0.00284	-0.04173	
0.00019	45 AP	5.907177	1	S	0.00000252	45	1	-0.00820	-0.00328
0.00015			X	0.00000704	45	2	-0.00162	-0.00259	
0.00025			Y	-0.00010548	45	3	0.01047	0.00437	-
0.00000			Z	0.00011929	45	4	0.00000	0.00000	
0.00314		2	S	-0.00005819	45	5	0.02474	-0.05500	
0.00313			X	0.00006799	45	6	0.02320	-0.05469	
0.00347			Y	-0.00005797	45	7	-0.02068	0.06070	-
0.00000			Z	0.00014635	45	8	0.00003	0.00002	
0.05698		3	S	-0.00009270	45	9	-0.01833	-0.99709	
0.03985			X	0.00001374	45	10	-0.00608	-0.69745	
0.06527			Y	0.00007271	45	11	0.01760	1.14220	-
0.00003			Z	-0.00805959	45	12	-0.00001	0.00050	-
0.02749		4	S	-0.00004602	45	13	-0.00831	-0.48112	
0.00060			X	-0.00004146	45	14	0.00905	-0.01046	
0.03831			Y	-0.00005416	45	15	-0.00299	0.67044	-
0.00001			Z	0.00309826	45	16	0.00004	0.00023	-
0.00103		5	S	0.00001228	45	17	-0.00005	-0.01795	
0.00003			X	0.00000682	45	18	-0.00127	-0.00059	
0.00155			Y	-0.00007438	45	19	-0.00386	0.02719	-
0.00000			Z	-0.00066258	45	20	0.00000	0.00001	
0.00010		6	S	0.00003541	45	21	0.00210	-0.00181	
0.00004			X	-0.00000740	45	22	0.00120	-0.00071	
0.00016			Y	0.00000687	45	23	-0.00128	0.00273	-
0.00000			Z	0.00019863	45	24	-0.00002	0.00000	
0.33634		7	S	-0.00003575	45	25	0.25680	-5.88604	
0.32213			X	-0.00007715	45	26	0.36878	-5.63727	
0.16473			Y	0.00016895	45	27	-0.20568	2.88278	-
0.00022			Z	0.07208604	45	28	-0.00025	0.00392	-
0.03192		8	S	0.00000156	45	29	0.00610	-0.99739	
0.03663			X	-0.00000411	45	30	-0.04615	-1.14482	
0.00107			Y	-0.00001103	45	31	0.03361	-0.03357	
0.00002			Z	-0.02231440	45	32	0.00003	0.00071	-

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00014		9	S	0.00002459	45	33	-0.00218	-0.00445		
			X	0.00004066	45	34	-0.00143	-0.00505		
0.00016			Y	0.00002238	45	35	0.00462	0.00284	-	
0.00009			Z	-0.00000389	45	36	-0.00001	0.00000		
0.00000		10	S	-0.00000328	45	37	-0.00043	-0.00001		
0.00000			X	0.00000593	45	38	0.00018	0.00000		
0.00000			Y	0.00001478	45	39	0.00090	0.00001		
0.00000			Z	-0.00003033	45	40	0.00000	0.00000		
0.00000		11	S	-0.00000361	45	41	-0.07476	-0.64899		
0.02077			X	-0.00004183	45	42	-0.00113	0.37888	-	
0.01212			Y	0.00001351	45	43	0.07128	0.65968	-	
0.02111			Z	0.00154613	45	44	0.00012	0.00036	-	
0.00001		12	S	0.00006978	45	45	1.04135	0.00000		
1.00000			X	-0.00073339	45	46	0.07141	0.00000		
0.00000			Y	-0.00011669	45	47	0.00614	0.00000		
0.00000			Z	-0.69910789	45	48	-0.00005	0.00000		
0.00000		13	S	-0.00000772	45	49	0.00802	-0.04606		
0.00312		14	S	-0.00000761	45	50	0.00031	-0.00006		
0.00000		15	S	0.00005336	45	51	0.00599	-0.00054		
0.00004		16	S	0.00002378	45	52	-0.00136	-0.00526		
0.00036		17	S	0.00002585	45	53	0.05001	-0.07887		
0.00535		18	S	0.00021043	45	54	0.49569	-7.48917		
0.50774		19	S	-0.50280428	45	55	0.49192	-7.48997		
0.50779		20	S	0.50265664	45	56	0.49192	-7.48967		
0.50777										
	46	A*		6.008560	1	S	-0.01077682	0.01100	0.00259	-
0.00015			X	-0.01344728	46	2	0.00049	0.00177	-	
0.00010			Y	0.25433421	46	3	-0.01483	-0.00359	-	
0.00021			Z	-0.00001587	46	4	0.00000	0.00000	-	
0.00000		2	S	0.12910266	46	5	-0.02497	0.05469	-	
0.00313			X	-0.16632842	46	6	-0.02088	0.04958	-	
0.00283			Y	0.14340471	46	7	0.01858	-0.06376	-	
0.00364			Z	-0.00001041	46	8	-0.00004	-0.00002	-	
0.00000		3	S	0.19350536	46	9	0.01631	0.69745	-	
0.03985			X	0.00635174	46	10	-0.00823	0.31782	-	
0.01816			Y	-0.04728536	46	11	-0.04180	-0.86908	-	
0.04966			Z	-0.00001009	46	12	0.00001	-0.00038	-	
0.00002		4	S	0.10932844	46	13	0.00212	0.01046	-	
0.00060			X	0.12516221	46	14	0.00334	-0.09070	-	
0.00518			Y	0.18363433	46	15	0.00379	-0.01570	-	
0.00090			Z	0.00000256	46	16	-0.00001	-0.00001	-	
0.00000		5	S	-0.02627115	46	17	-0.00101	0.00059	-	
0.00003			X	0.02563042	46	18	-0.00225	-0.00228	-	
0.00013			Y	0.26203588	46	19	-0.00537	-0.00094	-	
0.00005			Z	-0.00000030	46	20	0.00000	0.00000	-	
0.00000										

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00004		6	S	-0.08884480	46	21	0.00232	0.00071	-
			X	0.00999876	46	22	0.00401	0.00010	-
0.00001			Y	-0.01784385	46	23	-0.00069	-0.00112	
0.00006			Z	0.00000491	46	24	0.00002	0.00000	
0.00000		7	S	0.13493530	46	25	-0.46078	5.63727	-
0.32213			X	0.22073781	46	26	-0.52977	4.15282	-
0.23730			Y	-0.25608930	46	27	0.30860	-3.11233	
0.17785			Z	-0.00015763	46	28	0.00048	-0.00423	
0.00024		8	S	-0.02180580	46	29	-0.00773	1.54326	-
0.04938			X	-0.05555394	46	30	0.04813	1.73738	-
0.05560			Y	0.00308331	46	31	-0.00518	0.05634	-
0.00180			Z	0.00003708	46	32	-0.00007	-0.00119	
0.00004		9	S	-0.06582879	46	33	0.00074	0.00648	-
0.00021			X	-0.09197325	46	34	-0.00330	0.00722	-
0.00023			Y	-0.02962319	46	35	-0.00317	-0.00431	
0.00014			Z	-0.00002156	46	36	0.00001	0.00000	
0.00000		10	S	0.00515159	46	37	0.00053	0.00000	
0.00000			X	-0.01950157	46	38	-0.00009	0.00000	
0.00000			Y	-0.03715149	46	39	-0.00005	0.00000	
0.00000			Z	-0.00000390	46	40	0.00000	0.00000	
0.00000		11	S	-0.01255574	46	41	-0.08521	-0.50696	
0.01622			X	0.11129606	46	42	-0.00701	0.20731	-
0.00663			Y	0.04131208	46	43	0.05970	0.55587	-
0.01779			Z	0.00005619	46	44	0.00014	0.00030	-
0.00001		12	S	-0.02532873	46	45	0.07141	0.00000	
0.00000			X	0.18956842	46	46	0.98463	0.00000	
1.00000			Y	-0.49973083	46	47	0.06391	0.00000	
0.00000			Z	-0.00021289	46	48	0.00003	0.00000	
0.00000		13	S	0.04549611	46	49	-0.01112	0.06039	-
0.00409		14	S	0.02546925	46	50	-0.00068	0.00000	
0.00000		15	S	-0.12338423	46	51	-0.00674	0.00044	-
0.00003		16	S	-0.12262982	46	52	-0.00470	-0.00120	
0.00008		17	S	-0.10132696	46	53	0.06695	-0.06349	
0.00430		18	S	0.23156290	46	54	0.60997	-5.21045	
0.35325		19	S	-0.26630312	46	55	0.06441	-0.64073	
0.04344		20	S	-0.26617455	46	56	0.06537	-0.64844	
0.04396									
47	A*	6.228711	1	S	0.00755931	47	1	-0.00889	-0.00437
0.00025			X	0.04260154	47	2	-0.00050	-0.00359	
0.00021			Y	-0.17035431	47	3	0.00935	0.00569	-
0.00033			Z	0.00001438	47	4	0.00000	0.00000	
0.00000		2	S	-0.06930478	47	5	0.02820	-0.06070	
0.00347			X	0.10696457	47	6	0.02240	-0.06376	
0.00364			Y	-0.10570863	47	7	-0.01593	0.06288	-
0.00359			Z	0.00000779	47	8	0.00004	0.00002	
0.00000									

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.06527	3	S	-0.13379666	47	9	-0.02943	-1.14220	
		X	-0.01403946	47	10	0.01719	-0.86908	
0.04966		Y	-0.04897986	47	11	0.00645	1.21042	-
0.06917		Z	0.00001009	47	12	-0.00004	0.00063	-
0.00004	4	S	-0.02636538	47	13	0.00202	-0.67044	
0.03831		X	-0.17348683	47	14	0.00494	-0.01570	
0.00090		Y	-0.05581505	47	15	-0.02304	0.91510	-
0.05229		Z	-0.00000077	47	16	0.00003	0.00035	-
0.00002	5	S	0.01408064	47	17	0.00235	-0.02719	
0.00155		X	0.03942774	47	18	-0.00087	-0.00094	
0.00005		Y	-0.06182130	47	19	-0.00607	0.04092	-
0.00234		Z	0.00000205	47	20	0.00000	0.00001	
0.00000	6	S	0.04230486	47	21	0.00241	-0.00273	
0.00016		X	-0.00347596	47	22	0.00055	-0.00112	
0.00006		Y	0.01041496	47	23	-0.00175	0.00408	-
0.00023		Z	-0.00000219	47	24	-0.00002	0.00000	
0.00000	7	S	-0.12241481	47	25	0.23366	-2.88278	
0.16473		X	-0.12201560	47	26	0.29575	-3.11233	
0.17785		Y	0.16689850	47	27	-0.09431	-0.34174	
0.01953		Z	0.00007047	47	28	-0.00021	0.00216	-
0.00012	8	S	0.01506089	47	29	0.00967	0.04525	-
0.00145		X	0.02978432	47	30	-0.03286	0.05634	-
0.00180		Y	0.01070894	47	31	0.01561	-0.18253	
0.00584		Z	-0.00001069	47	32	0.00003	-0.00003	
0.00000	9	S	0.03141344	47	33	-0.00100	-0.00364	
0.00012		X	0.04651868	47	34	-0.00265	-0.00431	
0.00014		Y	0.02598237	47	35	0.00006	0.00198	-
0.00006		Z	0.00000767	47	36	-0.00001	0.00000	
0.00000	10	S	-0.00130466	47	37	-0.00035	-0.00001	
0.00000		X	0.01164577	47	38	0.00016	0.00000	
0.00000		Y	0.02034964	47	39	0.00086	0.00001	
0.00000		Z	0.00000266	47	40	0.00000	0.00000	
0.00000	11	S	0.07601945	47	41	-0.07489	-0.88268	
0.02825		X	0.08326415	47	42	-0.01609	0.55587	-
0.01779		Y	0.25228024	47	43	0.04310	0.85589	-
0.02739		Z	0.00010470	47	44	0.00012	0.00053	-
0.00002	12	S	-0.05006077	47	45	0.00614	0.00000	
0.00000		X	-0.48940572	47	46	0.06391	0.00000	
0.00000		Y	-0.28696281	47	47	1.03273	0.00000	
1.00000		Z	0.00062343	47	48	-0.00004	0.00000	
0.00000	13	S	-0.01528305	47	49	0.00295	-0.01837	
0.00125	14	S	-0.01731857	47	50	0.00030	-0.00008	
0.00001	15	S	0.10411745	47	51	0.00576	-0.00062	
0.00004	16	S	0.00893707	47	52	-0.00039	-0.00727	
0.00049	17	S	-0.24081065	47	53	0.06736	-0.08637	
0.00586								



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.32848		18	S	0.57503510	47	54	0.57008	-4.84502	
		19	S	-0.08819012	47	55	-0.50079	4.08499	-
0.27695		20	S	-0.08858757	47	56	-0.50079	4.08506	-
0.27695									
48	A*	6.664718							
0.00000		1	S	0.03323083	48	1	-0.00001	0.00000	
			X	0.22871627	48	2	0.00000	0.00000	
0.00000			Y	-0.02869995	48	3	0.00001	0.00000	
0.00000			Z	0.00003187	48	4	0.00122	-0.00036	
0.00002		2	S	0.04129053	48	5	0.00003	-0.00002	
0.00000			X	0.02602667	48	6	0.00002	-0.00002	
0.00000			Y	-0.10670351	48	7	-0.00002	0.00002	
0.00000			Z	0.00000439	48	8	-0.02174	-0.00788	
0.00045		3	S	0.00533328	48	9	-0.00002	-0.00050	
0.00003			X	0.17134896	48	10	0.00000	-0.00038	
0.00002			Y	0.01745504	48	11	0.00003	0.00063	-
0.00004			Z	0.00001405	48	12	-0.01256	-0.21286	
0.01216		4	S	-0.03280728	48	13	0.00000	-0.00023	
0.00001			X	0.02600502	48	14	0.00001	-0.00001	
0.00000			Y	0.14662749	48	15	-0.00001	0.00035	-
0.00002			Z	-0.00001171	48	16	-0.01718	-0.09094	
0.00520		5	S	-0.07162920	48	17	0.00000	-0.00001	
0.00000			X	0.35880885	48	18	0.00000	0.00000	
0.00000			Y	0.08476494	48	19	0.00000	0.00001	
0.00000			Z	0.00003671	48	20	0.00253	-0.00230	
0.00013		6	S	0.01218880	48	21	0.00000	0.00000	
0.00000			X	0.25026867	48	22	0.00000	0.00000	
0.00000			Y	-0.14757255	48	23	0.00000	0.00000	
0.00000			Z	0.00001064	48	24	0.01358	-0.00019	
0.00001		7	S	0.00976092	48	25	0.00032	-0.00392	
0.00022			X	-0.00757470	48	26	0.00049	-0.00423	
0.00024			Y	0.00508861	48	27	-0.00022	0.00216	-
0.00012			Z	-0.00000268	48	28	0.18895	-1.93332	
0.11048		8	S	0.00078327	48	29	0.00001	-0.00096	
0.00003			X	-0.00516760	48	30	-0.00008	-0.00119	
0.00004			Y	0.00148736	48	31	0.00001	-0.00003	
0.00000			Z	0.00000167	48	32	-0.08262	-0.18419	
0.00589		9	S	-0.00187610	48	33	0.00000	0.00000	
0.00000			X	-0.02248181	48	34	0.00000	0.00000	
0.00000			Y	-0.02474253	48	35	0.00001	0.00000	
0.00000			Z	0.00000766	48	36	0.00513	-0.00045	
0.00001		10	S	0.26599506	48	37	0.00000	0.00000	
0.00000			X	0.38705441	48	38	0.00000	0.00000	
0.00000			Y	0.05965188	48	39	0.00000	0.00000	
0.00000			Z	0.00011790	48	40	-0.00323	0.00000	
0.00000		11	S	0.00598344	48	41	0.00007	-0.00048	
0.00002									

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00001		X	-0.04895877	48	42	-0.00001	0.00030	-			
0.00002		Y	-0.01812967	48	43	-0.00008	0.00053	-			
0.00358		Z	-0.00000929	48	44	0.00665	-0.11195				
0.00000	12	S	0.00701306	48	45	-0.00005	0.00000				
0.00000		X	0.01796019	48	46	0.00003	0.00000				
0.00000		Y	0.01550421	48	47	-0.00004	0.00000				
0.00000		Z	-0.00001303	48	48	1.01654	0.00000				
1.00000	13	S	-0.02871905	48	49	0.00001	-0.00002				
0.00000	14	S	-0.58015978	48	50	0.00000	0.00000				
0.00000	15	S	0.17949694	48	51	0.00001	0.00000				
0.00000	16	S	-0.23021066	48	52	0.00000	0.00000				
0.00000	17	S	0.03240338	48	53	-0.00004	-0.00003				
0.00000	18	S	-0.02974921	48	54	-0.00042	0.00358	-			
0.00024	19	S	0.00446818	48	55	-0.69142	5.79076	-			
0.39259	20	S	0.00446960	48	56	0.69133	-5.78968				
0.39252											
0.00926	49	A*	6.830652	1	S	-0.05843802	49	1	0.03775	-0.13654	
0.00436		X	-0.30727381	49	2	-0.00590	0.06431	-			
0.01167		Y	0.06424097	49	3	-0.03524	0.17207	-			
0.00000		Z	-0.00003924	49	4	-0.00003	-0.00002				
0.11118	2	S	-0.03560030	49	5	-0.00079	-1.63994				
0.07606		X	-0.04727393	49	6	0.02142	1.12189	-			
0.11265		Y	0.13232988	49	7	-0.00268	1.66151	-			
0.00003		Z	-0.00000626	49	8	0.00004	-0.00039				
0.04084	3	S	-0.00450827	49	9	-0.01632	-0.60242				
0.04868		X	-0.26703823	49	10	0.00026	0.71810	-			
0.02009		Y	-0.10351263	49	11	-0.00816	0.29634	-			
0.00000		Z	-0.00002064	49	12	-0.00001	-0.00007				
0.00217	4	S	0.03685293	49	13	0.00561	-0.03200				
0.00270		X	-0.05720252	49	14	-0.00464	0.03990	-			
0.00127		Y	-0.31560671	49	15	-0.00415	0.01870	-			
0.00000		Z	0.00001988	49	16	0.00001	0.00000				
0.00042	5	S	0.08318568	49	17	0.00056	-0.00619				
0.00044		X	-0.24193922	49	18	-0.00228	0.00653	-			
0.00039		Y	-0.22776006	49	19	0.00187	0.00570	-			
0.00000		Z	-0.00001875	49	20	0.00001	0.00000				
0.00069	6	S	0.04368965	49	21	-0.01399	-0.01011				
0.00050		X	-0.22883078	49	22	0.01381	0.00737	-			
0.00081		Y	-0.07505005	49	23	0.00604	0.01202	-			
0.00000		Z	-0.00001437	49	24	-0.00001	0.00000				
0.05415	7	S	-0.01317189	49	25	0.01143	-0.79877				
0.06775		X	0.07141247	49	26	-0.01096	0.99927	-			
0.01309		Y	-0.09079333	49	27	0.01186	-0.19305				
0.00001		Z	-0.00003919	49	28	-0.00003	-0.00012				
0.09751	8	S	0.00030998	49	29	0.09156	-2.77905				

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.07321		X	0.00805496	49	30	-0.14527	2.08650	-
		Y	0.00630392	49	31	0.11482	-1.86732	
0.06552		Z	-0.00000050	49	32	-0.00002	0.00046	-
0.00002								
0.38420	9	S	-0.01262669	49	33	0.45358	-10.94972	
0.04367		X	0.01060367	49	34	0.12993	-1.24448	
0.32488		Y	0.03521446	49	35	-0.82702	9.25903	-
0.00015		Z	-0.00001674	49	36	0.00039	-0.00438	
0.00001	10	S	0.19271778	49	37	0.00316	-0.00025	
0.00000		X	0.33588260	49	38	-0.00054	0.00011	
0.00001		Y	0.08325095	49	39	-0.00589	0.00026	-
0.00000		Z	0.00009243	49	40	0.00000	0.00000	
0.00000	11	S	-0.01391825	49	41	0.00015	-0.00157	
0.00005		X	0.09779835	49	42	0.00076	0.00170	-
0.00006		Y	0.01611482	49	43	-0.00091	0.00037	-
0.00001		Z	0.00000954	49	44	0.00000	0.00000	
0.00000	12	S	-0.01913376	49	45	0.00802	-0.04606	
0.00312		X	0.05621102	49	46	-0.01112	0.06039	-
0.00409		Y	-0.05703696	49	47	0.00295	-0.01837	
0.00125		Z	-0.00005489	49	48	0.00001	-0.00002	
0.00000	13	S	0.05352038	49	49	0.78535	0.00000	
1.00000	14	S	-0.45800477	49	50	-0.00240	-0.00013	
0.00001	15	S	-0.21523209	49	51	0.00318	-0.06131	
0.00511	16	S	0.24628218	49	52	-0.00013	-0.00076	
0.00006	17	S	-0.05923028	49	53	0.00022	-0.00040	
0.00003	18	S	0.01070882	49	54	-0.00397	-0.01182	
0.00099	19	S	-0.02700715	49	55	0.00172	-0.01880	
0.00157	20	S	-0.02698602	49	56	0.00173	-0.01878	
0.00157								
50	A*							
0.00892	7.105062	1	S	0.08312505	50	1	0.03817	-0.13163
0.00779		X	0.24251994	50	2	0.03031	-0.11485	
0.00915		Y	-0.23138979	50	3	0.02567	-0.13498	
0.00000		Z	0.00003848	50	4	-0.00001	-0.00001	
0.00069		2	S	0.00237986	50	5	-0.01239	-0.01014
0.00046		X	0.09903938	50	6	0.00103	-0.00682	
0.00084		Y	-0.25981596	50	7	-0.01505	-0.01238	
0.00000		Z	0.00001246	50	8	0.00000	0.00000	
0.00041		3	S	-0.03445208	50	9	0.00108	-0.00599
0.00011		X	-0.00222516	50	10	-0.00190	-0.00166	
0.00056		Y	-0.41573292	50	11	0.00174	-0.00822	
0.00000		Z	0.00001177	50	12	0.00001	0.00000	
0.00236		4	S	-0.03197826	50	13	0.00427	-0.03474
0.00024		X	-0.11992761	50	14	-0.00014	0.00360	-
0.00323		Y	-0.26968241	50	15	0.00340	-0.04766	
0.00000		Z	0.00000294	50	16	0.00000	0.00000	
0.04387		5	S	0.03095249	50	17	-0.00991	-0.64708

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00556		X	0.04836074	50	18	0.01836	0.08195	-			
		Y	-0.31797469	50	19	0.01284	-0.82799				
0.05614		Z	0.00001058	50	20	-0.00001	-0.00004				
0.00000											
0.11207	6	S	0.06270376	50	21	-0.00212	-1.65306				
0.06462		X	0.17612007	50	22	0.01052	-0.95322				
0.12072		Y	0.12659290	50	23	-0.01748	-1.78059				
0.00001		Z	0.00000329	50	24	0.00001	-0.00020				
0.00002	7	S	-0.04036694	50	25	-0.00055	-0.00023				
0.00000		X	0.24191284	50	26	0.00033	-0.00005				
0.00002		Y	-0.34737188	50	27	-0.00089	-0.00033				
0.00000		Z	-0.00016580	50	28	0.00000	0.00000				
0.00000											
0.00000	8	S	0.01830891	50	29	0.00014	-0.00001				
0.00000		X	0.00407265	50	30	-0.00058	0.00000				
0.00000		Y	0.05046478	50	31	0.00030	-0.00001				
0.00000		Z	-0.00000184	50	32	0.00000	0.00000				
0.00000											
0.00001	9	S	-0.00153493	50	33	0.00296	-0.00026				
0.00001		X	-0.02915223	50	34	0.00461	-0.00018				
0.00001		Y	-0.01909530	50	35	0.00345	-0.00024				
0.00000		Z	0.00000779	50	36	0.00000	0.00000				
0.38752	10	S	-0.07527000	50	37	0.45846	-11.04438				
0.30956		X	-0.06306525	50	38	0.82015	-8.82232				
0.11413		Y	0.06796175	50	39	0.27714	-3.25283				
0.00009		Z	-0.00001999	50	40	0.00023	-0.00247				
0.00009	11	S	0.00703966	50	41	-0.00077	-0.00246				
0.00003		X	0.01736424	50	42	0.00046	0.00090	-			
0.00009		Y	0.00015610	50	43	-0.00137	-0.00258				
0.00000		Z	-0.00001652	50	44	0.00000	0.00000				
0.00000											
0.00000	12	S	-0.05083924	50	45	0.00031	-0.00006				
0.00000		X	0.27974927	50	46	-0.00068	0.00000				
0.00001		Y	-0.15347302	50	47	0.00030	-0.00008				
0.00000		Z	-0.00024373	50	48	0.00000	0.00000				
0.00001	13	S	-0.03400427	50	49	-0.00240	-0.00013				
1.00000	14	S	0.07639278	50	50	0.81292	0.00000				
0.00469	15	S	0.22530635	50	51	0.00151	-0.05626				
0.06109	16	S	0.07301991	50	52	0.02886	-0.73306				
0.00071	17	S	-0.01080053	50	53	-0.00009	-0.00857				
0.00003	18	S	-0.07705245	50	54	0.00015	-0.00031				
0.00000	19	S	-0.07999822	50	55	-0.00017	-0.00002				
0.00000	20	S	-0.07993148	50	56	-0.00017	-0.00002				
0.51331	51	A*	7.370121	1	S	0.00056196	51	1	0.56042	-7.57130	
0.42207		X	0.23111956	51	2	-0.71098	6.22548	-			
0.23991		Y	0.41668326	51	3	0.40225	-3.53874				
0.00008		Z	0.00001250	51	4	-0.00013	0.00124	-			
0.09778											
	2	S	0.02633664	51	5	-0.01829	-1.44222				

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.04943		X	-0.20033598	51	6	-0.00252	0.72915	-
		Y	0.36790010	51	7	-0.04357	-1.62247	
0.11000		Z	-0.00002490	51	8	-0.00001	0.00016	-
0.00001	3	S	0.00919737	51	9	0.04290	-0.12263	
0.00831		X	-0.33613631	51	10	-0.03823	0.10348	-
0.00702		Y	0.10048460	51	11	0.02922	-0.12896	
0.00874		Z	-0.00003228	51	12	0.00000	0.00002	
0.00000	4	S	-0.01873630	51	13	0.00672	-0.04375	
0.00297		X	-0.11685718	51	14	-0.00313	0.05208	-
0.00353		Y	-0.26704416	51	15	0.00333	-0.02979	
0.00202		Z	0.00001068	51	16	0.00001	0.00001	
0.00000	5	S	-0.02585261	51	17	0.04283	-0.13178	
0.00893		X	0.24939568	51	18	-0.04497	0.17547	-
0.01190		Y	-0.30519649	51	19	0.01669	-0.02622	
0.00178		Z	0.00002521	51	20	0.00000	0.00002	
0.00000	6	S	-0.02029402	51	21	-0.01562	-1.45775	
0.09883		X	0.43852431	51	22	0.03763	1.78445	-
0.12098		Y	-0.01633591	51	23	0.02277	0.20918	-
0.01418		Z	0.00002686	51	24	-0.00001	0.00021	-
0.00001	7	S	0.00151358	51	25	-0.01627	-0.00877	
0.00059		X	-0.04850141	51	26	0.00308	0.00563	-
0.00038		Y	0.08970410	51	27	-0.02264	-0.01086	
0.00074		Z	0.00004290	51	28	-0.00001	0.00000	
0.00000	8	S	-0.00349042	51	29	-0.00039	-0.00213	
0.00007		X	0.00922216	51	30	-0.00052	0.00050	-
0.00002		Y	-0.01361543	51	31	0.00442	-0.00231	
0.00008		Z	-0.00000368	51	32	0.00001	0.00000	
0.00000	9	S	-0.01957390	51	33	-0.00625	-0.44916	
0.01576		X	-0.00085657	51	34	-0.01858	-0.07579	
0.00266		Y	0.01579769	51	35	0.00647	-0.47552	
0.01668		Z	-0.00001462	51	36	0.00000	0.00002	
0.00000	10	S	-0.02217507	51	37	-0.00607	-0.39553	
0.01388		X	-0.07313558	51	38	-0.01228	0.33082	-
0.01161		Y	-0.03636113	51	39	0.01393	0.26681	-
0.00936		Z	-0.00001557	51	40	0.00000	0.00003	
0.00000	11	S	0.00254527	51	41	0.00049	-0.00084	
0.00003		X	0.02387312	51	42	0.00212	0.00082	-
0.00003		Y	0.01969643	51	43	0.00127	-0.00045	
0.00002		Z	0.00000445	51	44	0.00000	0.00000	
0.00000	12	S	0.01353376	51	45	0.00599	-0.00054	
0.00004		X	-0.07652732	51	46	-0.00674	0.00044	-
0.00003		Y	0.03959480	51	47	0.00576	-0.00062	
0.00004		Z	0.00005100	51	48	0.00001	0.00000	
0.00000	13	S	0.04884860	51	49	0.00318	-0.06131	
0.00511	14	S	0.07903928	51	50	0.00151	-0.05626	
0.00469								

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

1.00000		15	S	-0.00314596	51	51	0.94300	0.00000
0.00168		16	S	-0.04188169	51	52	-0.02911	-0.02015
0.00006		17	S	-0.02445859	51	53	-0.00047	-0.00067
0.00006		18	S	0.02118732	51	54	0.00119	-0.00071
0.00002		19	S	0.02001394	51	55	-0.00306	-0.00018
0.00002		20	S	0.02001528	51	56	-0.00305	-0.00018
0.00897	52 A* 7.578414	1	S	0.04563970	52	1	0.04103	-0.13238
0.01193			X	0.10569972	52	2	0.04538	-0.17596
0.00192			Y	-0.14593573	52	3	0.01641	-0.02825
0.00000			Z	0.00001367	52	4	0.00000	-0.00002
0.00304		2	S	0.01193392	52	5	0.00916	-0.04490
0.00360			X	-0.30946681	52	6	0.00377	-0.05306
0.00212			Y	-0.23389140	52	7	0.00369	-0.03121
0.00000			Z	-0.00001240	52	8	-0.00002	0.00000
0.00842		3	S	0.03982118	52	9	0.04183	-0.12413
0.00698			X	-0.00467481	52	10	0.03655	-0.10289
0.00895			Y	0.15692148	52	11	0.02769	-0.13195
0.00000			Z	-0.00001232	52	12	0.00000	-0.00001
0.09781		4	S	0.01137261	52	13	-0.01577	-1.44273
0.04752			X	0.14802989	52	14	0.00413	-0.70091
0.11088			Y	-0.05938529	52	15	-0.04678	-1.63551
0.00000			Z	0.00002204	52	16	0.00001	-0.00005
0.51329		5	S	0.01869290	52	17	0.55595	-7.57107
0.41838			X	-0.05129606	52	18	0.70843	-6.17109
0.24628			Y	-0.03378269	52	19	0.41265	-3.63262
0.00006			Z	-0.00000412	52	20	0.00010	-0.00093
0.09944		6	S	0.01078801	52	21	-0.01405	-1.46669
0.12183			X	-0.01084128	52	22	-0.04000	-1.79697
0.01286			Y	0.08546972	52	23	0.02235	0.18967
0.00001			Z	-0.00000416	52	24	0.00001	-0.00019
0.00059		7	S	0.03033929	52	25	-0.01750	-0.00875
0.00037			X	-0.04500079	52	26	0.00000	-0.00550
0.00074			Y	0.05652663	52	27	-0.02207	-0.01091
0.00000			Z	0.00002522	52	28	0.00000	0.00000
0.00001		8	S	-0.06127745	52	29	0.00175	-0.00028
0.00001			X	0.05952693	52	30	0.00309	-0.00017
0.00001			Y	-0.08314352	52	31	0.00975	-0.00027
0.00000			Z	0.00003409	52	32	-0.00001	0.00000
0.00003		9	S	-0.35964447	52	33	0.00008	-0.00087
0.00003			X	-0.28221315	52	34	-0.00205	-0.00084
0.00002			Y	0.32246754	52	35	-0.00102	-0.00048
0.00000			Z	-0.00022272	52	36	0.00000	0.00000
0.01416		10	S	-0.02244623	52	37	-0.01632	-0.40362
0.01193			X	0.00991558	52	38	-0.00437	-0.33991

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00944		Y	0.05718806	52	39	0.00944	0.26912	-
0.00000		Z	0.00000010	52	40	-0.00001	-0.00005	
0.01626		11 S	-0.04253671	52	41	-0.01669	-0.46333	
0.00313		X	0.10561316	52	42	0.00622	0.08923	-
0.01713		Y	-0.02827366	52	43	-0.00880	-0.48833	
0.00000		Z	0.00001577	52	44	0.00000	0.00003	
0.00036		12 S	0.00809468	52	45	-0.00136	-0.00526	
0.00008		X	-0.02967652	52	46	-0.00470	-0.00120	
0.00049		Y	0.02220119	52	47	-0.00039	-0.00727	
0.00000		Z	0.00003440	52	48	0.00000	0.00000	
0.00006		13 S	0.62410194	52	49	-0.00013	-0.00076	
0.06109		14 S	-0.01621295	52	50	0.02886	-0.73306	
0.00168		15 S	0.08277448	52	51	-0.02911	-0.02015	
1.00000		16 S	0.03127278	52	52	0.95986	0.00000	
0.06250		17 S	-0.03381754	52	53	0.03228	-0.74999	
0.00217		18 S	0.00801556	52	54	0.00142	-0.02604	
0.00012		19 S	0.00907529	52	55	0.00015	-0.00143	
0.00012		20 S	0.00905862	52	56	0.00015	-0.00143	
0.00036	53 A*	7.741604	1 S	0.03587813	53	1	0.00007	-0.00529
0.00048		X	0.12360445	53	2	0.00057	-0.00712	
0.00014		Y	-0.00601413	53	3	-0.00121	0.00206	-
0.00000		Z	0.00001481	53	4	0.00000	0.00000	
0.00052		2 S	0.04490541	53	5	-0.01134	-0.00769	
0.00073		X	-0.06984551	53	6	-0.01122	-0.01075	
0.00001		Y	-0.04899070	53	7	0.00765	-0.00019	
0.00000		Z	-0.00000965	53	8	0.00000	0.00000	
0.00644		3 S	0.07694948	53	9	0.03311	-0.09506	
0.00851		X	0.16702260	53	10	0.04258	-0.12549	
0.00196		Y	0.21866298	53	11	0.02041	-0.02897	
0.00000		Z	0.00000401	53	12	0.00001	-0.00001	
0.08847		4 S	0.03776037	53	13	-0.01591	-1.30498	
0.10976		X	0.56788576	53	14	-0.03518	-1.61894	
0.00362		Y	-0.20614852	53	15	0.01940	-0.05334	
0.00001		Z	0.00007852	53	16	-0.00001	-0.00013	
0.03988		5 S	0.04698181	53	17	-0.01138	-0.58820	
0.04394		X	-0.10935301	53	18	0.02215	-0.64806	
0.02682		Y	-0.13484293	53	19	0.01056	0.39552	-
0.00000		Z	-0.00000752	53	20	0.00001	-0.00007	
0.00213		6 S	0.02358287	53	21	0.00441	-0.03143	
0.00251		X	0.05327493	53	22	0.00241	-0.03696	
0.00153		Y	0.22376238	53	23	-0.00129	0.02255	-
0.00000		Z	-0.00000631	53	24	0.00000	0.00000	
0.00188		7 S	0.04291578	53	25	-0.00236	-0.02776	
0.00217		X	-0.05576235	53	26	-0.00274	-0.03202	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00142		Y	0.09086615	53	27	-0.00335	-0.02101			
0.00000		Z	0.00002686	53	28	0.00001	0.00000			
0.00003	8	S	0.01849656	53	29	0.00263	-0.00074			
0.00002		X	-0.04258943	53	30	0.00658	-0.00068			
0.00002		Y	0.01903802	53	31	0.00177	-0.00045			
0.00000		Z	-0.00000677	53	32	-0.00001	0.00000			
0.00001	9	S	0.08050073	53	33	0.00225	-0.00017			
0.00001		X	-0.02991789	53	34	0.00811	-0.00018			
0.00000		Y	-0.24494259	53	35	0.00021	-0.00002			
0.00000		Z	0.00009803	53	36	0.00000	0.00000			
0.00007	10	S	-0.05782856	53	37	-0.00086	-0.00210			
0.00006		X	0.03095776	53	38	-0.00089	-0.00162			
0.00006		Y	0.15666068	53	39	0.00105	0.00167	-		
0.00000		Z	0.00000172	53	40	0.00000	0.00000			
0.33799	11	S	-0.16349293	53	41	0.42924	-9.63264			
0.23093		X	0.40023693	53	42	0.63344	-6.58164			
0.18646		Y	-0.10901298	53	43	0.59877	-5.31399			
0.00001		Z	0.00006172	53	44	-0.00003	0.00032	-		
0.00535	12	S	0.00675390	53	45	0.05001	-0.07887			
0.00430		X	-0.05370951	53	46	0.06695	-0.06349			
0.00586		Y	-0.00802792	53	47	0.06736	-0.08637			
0.00000		Z	0.00006346	53	48	-0.00004	-0.00003			
0.00003	13	S	-0.31084114	53	49	0.00022	-0.00040			
0.00071	14	S	-0.05162380	53	50	-0.00009	-0.00857			
0.00006	15	S	0.06421449	53	51	-0.00047	-0.00067			
0.06250	16	S	0.07469936	53	52	0.03228	-0.74999			
1.00000	17	S	-0.12603284	53	53	0.80968	0.00000			
0.03768	18	S	0.04031226	53	54	0.01898	-0.45213			
0.00193	19	S	0.00073827	53	55	-0.01455	-0.02312			
0.00193	20	S	0.00070599	53	56	-0.01451	-0.02317			
0.00037	54 A*	8.115330	1	S	-0.03884998	54	1	-0.00112	-0.00548	
0.00035				X	-0.19313964	54	2	0.00076	-0.00522	
0.00038				Y	-0.08927497	54	3	0.00132	0.00564	-
0.00000				Z	-0.00001793	54	4	-0.00001	0.00000	
0.00272			2	S	-0.02257172	54	5	0.01103	-0.04013	
0.00314				X	0.15983206	54	6	0.01018	-0.04638	
0.00202				Y	-0.07259668	54	7	-0.00610	0.02974	-
0.00000				Z	0.00001723	54	8	0.00002	0.00002	
0.05039			3	S	-0.00359044	54	9	-0.01820	-0.74321	
0.05309				X	0.13986693	54	10	0.00846	-0.78306	
0.03647				Y	-0.00833181	54	11	-0.00021	0.53794	-
0.00004				Z	0.00000995	54	12	-0.00001	0.00056	-
0.07476			4	S	-0.01143774	54	13	0.00895	-1.10278	
0.03310				X	0.26523894	54	14	0.00310	-0.48830	



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.08768		Y	-0.18285251	54	15	-0.02262	1.29329	-
		Z	0.00004151	54	16	-0.00003	0.00092	-
0.00006								
0.00477	5	S	-0.03404590	54	17	0.01166	-0.07038	
		X	0.19461460	54	18	0.00219	-0.02230	
0.00151								
0.00632		Y	-0.17524908	54	19	-0.01334	0.09321	-
		Z	0.00001537	54	20	0.00002	0.00004	
0.00000								
0.00042	6	S	-0.01695924	54	21	-0.00191	-0.00624	
		X	0.04261247	54	22	-0.00225	-0.00379	
0.00026								
0.00053		Y	-0.63094032	54	23	0.00050	0.00787	-
		Z	0.00002889	54	24	-0.00001	0.00000	
0.00000								
0.11197	7	S	-0.00041888	54	25	-0.00541	-1.65149	
		X	0.01230458	54	26	-0.00397	-2.01736	
0.13677								
0.00315		Y	-0.02101723	54	27	0.00150	-0.04650	
		Z	-0.00002096	54	28	-0.00001	0.00140	-
0.00009								
0.00431	8	S	-0.00395398	54	29	0.02146	-0.12280	
		X	0.01178183	54	30	0.05181	-0.13005	
0.00456								
0.00113		Y	-0.00178882	54	31	-0.00172	-0.03232	
		Z	0.00000505	54	32	-0.00002	0.00008	
0.00000								
0.00010	9	S	0.00797619	54	33	0.00186	-0.00291	
		X	0.05611188	54	34	-0.00126	-0.00308	
0.00011								
0.00003		Y	0.09409138	54	35	-0.00523	0.00097	-
		Z	-0.00002239	54	36	0.00000	0.00000	
0.00000								
0.00000	10	S	0.15484950	54	37	0.00043	-0.00013	
		X	-0.10058083	54	38	0.00056	-0.00005	
0.00000								
0.00000		Y	-0.43336049	54	39	-0.00118	0.00014	
		Z	-0.00000780	54	40	0.00000	0.00000	
0.00000								
0.14724	11	S	-0.08411138	54	41	0.09151	-4.19636	
		X	0.20564000	54	42	-0.03963	1.31518	-
0.04615								
0.13653		Y	-0.05913426	54	43	-0.18713	3.89121	-
		Z	0.00002777	54	44	-0.00024	0.00449	-
0.00016								
0.50774	12	S	-0.00630182	54	45	0.49569	-7.48917	
		X	0.02079485	54	46	0.60997	-5.21045	
0.35325								
0.32848		Y	-0.02637628	54	47	0.57008	-4.84502	
		Z	-0.00000765	54	48	-0.00042	0.00358	-
0.00024								
0.00099	13	S	0.08266128	54	49	-0.00397	-0.01182	
0.00003	14	S	0.15743764	54	50	0.00015	-0.00031	
0.00006	15	S	-0.04861561	54	51	0.00119	-0.00071	
0.00217	16	S	-0.03648350	54	52	0.00142	-0.02604	
0.03768	17	S	-0.06410175	54	53	0.01898	-0.45213	
1.00000	18	S	0.00188004	54	54	0.91608	0.00000	
0.17775	19	S	-0.01066275	54	55	-0.00226	-2.13299	
0.17773	20	S	-0.01067031	54	56	-0.00228	-2.13281	
55	A*							
0.00007	8.340780	1	S	-0.01142719	55	1	0.00415	-0.00103
0.00005		X	0.05892529	55	2	0.00064	-0.00069	

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00009		Y	0.19647323	55	3	-0.00472	0.00127	-
0.00002		Z	0.00000026	55	4	-0.00308	0.00022	-
0.00097	2	S	-0.04142185	55	5	-0.01050	-0.01430	
0.00081		X	0.55444437	55	6	-0.01044	-0.01191	
0.00105		Y	0.26153821	55	7	0.00703	0.01543	-
0.00026		Z	0.00005005	55	8	0.02105	0.00381	-
0.01352	3	S	-0.03637657	55	9	0.02907	-0.19942	
0.00791		X	0.21665554	55	10	0.00416	-0.11664	
0.01548		Y	-0.08359604	55	11	-0.02816	0.22829	-
0.00482		Z	0.00001978	55	12	0.02622	0.07115	-
0.00622	4	S	-0.00341580	55	13	0.00268	-0.09175	
0.00033		X	0.18077193	55	14	-0.00102	-0.00484	
0.00818		Y	0.01065513	55	15	-0.00035	0.12067	-
0.00202		Z	0.00001820	55	16	0.01989	0.02972	-
0.00029	5	S	0.00776472	55	17	-0.00082	-0.00435	
0.00002		X	-0.03705518	55	18	0.00044	-0.00023	
0.00041		Y	0.00681558	55	19	0.00239	0.00601	-
0.00007		Z	-0.00000177	55	20	-0.00340	0.00104	-
0.00004	6	S	-0.00353284	55	21	0.00001	-0.00056	
0.00001		X	0.07536184	55	22	0.00016	-0.00019	
0.00005		Y	0.22715101	55	23	0.00013	0.00077	-
0.00001		Z	-0.00000414	55	24	-0.01455	0.00012	-
0.11196	7	S	-0.00998500	55	25	-0.00074	-1.65148	
0.09229		X	-0.00026004	55	26	-0.00221	-1.36127	
0.08376		Y	-0.02470884	55	27	0.00029	1.23548	-
0.05641		Z	-0.00002443	55	28	-0.11002	0.83212	-
0.01552	8	S	-0.02188866	55	29	-0.00089	-0.44240	
0.01543		X	0.03495065	55	30	0.00017	-0.43962	
0.00331		Y	-0.02047072	55	31	-0.00697	0.09422	-
0.00531		Z	0.00001613	55	32	0.07990	0.15141	-
0.00009	9	S	0.09866513	55	33	-0.00031	-0.00257	
0.00008		X	0.33557528	55	34	0.00201	-0.00230	
0.00006		Y	0.40485942	55	35	0.00052	0.00161	-
0.00002		Z	-0.00007566	55	36	-0.00588	0.00050	-
0.00000	10	S	-0.05871652	55	37	0.00005	-0.00001	
0.00000		X	0.02544631	55	38	-0.00017	0.00000	
0.00000		Y	0.15004627	55	39	0.00006	0.00001	
0.00000		Z	0.00000057	55	40	0.00361	0.00000	
0.00501	11	S	-0.04319855	55	41	0.01395	-0.14278	
0.00203		X	0.09366457	55	42	-0.00035	0.05789	-
0.00485		Y	-0.03515258	55	43	-0.00844	0.13823	-
0.00146		Z	0.00001302	55	44	-0.00285	0.04174	-
0.50779	12	S	-0.00324386	55	45	0.49192	-7.48997	
0.04344		X	0.01807972	55	46	0.06441	-0.64073	
0.27695		Y	-0.01770553	55	47	-0.50079	4.08499	-

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.39259		Z	-0.00000444	55	48	-0.69142	5.79076	-	
0.00157		13 S	0.31966013	55	49	0.00172	-0.01880		
0.00000		14 S	-0.04585098	55	50	-0.00017	-0.00002		
0.00002		15 S	-0.01629312	55	51	-0.00306	-0.00018		
0.00012		16 S	0.00298131	55	52	0.00015	-0.00143		
0.00193		17 S	-0.02311345	55	53	-0.01455	-0.02312		
0.17775		18 S	-0.00215785	55	54	-0.00226	-2.13299		
1.00000		19 S	-0.00790461	55	55	0.95537	0.00000		
0.17779		20 S	-0.00791167	55	56	0.01355	-2.13354		
0.00007	56 A*	11.613201	1 S	0.00088595	56	1	0.00415	-0.00103	
0.00005			X	0.00281805	56	2	0.00063	-0.00069	
0.00009			Y	-0.00513988	56	3	-0.00471	0.00127	-
0.00001			Z	0.00000024	56	4	0.00309	-0.00022	
0.00097			2 S	0.00658014	56	5	-0.01049	-0.01428	
0.00081			X	0.00720006	56	6	-0.01042	-0.01190	
0.00105			Y	-0.00014540	56	7	0.00701	0.01542	-
0.00026			Z	0.00000415	56	8	-0.02109	-0.00380	
0.01352			3 S	0.05104484	56	9	0.02906	-0.19942	
0.00791			X	0.01412313	56	10	0.00414	-0.11674	
0.01548			Y	-0.12583515	56	11	-0.02816	0.22829	-
0.00481			Z	-0.00001888	56	12	-0.02622	-0.07099	
0.00623			4 S	0.01177301	56	13	0.00267	-0.09183	
0.00033			X	-0.02537447	56	14	-0.00101	-0.00489	
0.00819			Y	-0.03128256	56	15	-0.00035	0.12079	-
0.00201			Z	0.00000122	56	16	-0.01992	-0.02968	
0.00030			5 S	0.00658663	56	17	-0.00082	-0.00435	
0.00002			X	-0.00069418	56	18	0.00044	-0.00023	
0.00041			Y	-0.01720270	56	19	0.00238	0.00601	-
0.00007			Z	0.00000046	56	20	0.00340	-0.00104	
0.00004			6 S	0.00121770	56	21	0.00001	-0.00056	
0.00001			X	0.00193972	56	22	0.00016	-0.00019	
0.00005			Y	-0.00409288	56	23	0.00013	0.00077	-
0.00001			Z	0.00000005	56	24	0.01457	-0.00012	
0.11196			7 S	0.23074989	56	25	-0.00074	-1.65146	
0.09236			X	-0.55589664	56	26	-0.00208	-1.36237	
0.08376			Y	-0.38771075	56	27	0.00027	1.23550	-
0.05629			Z	0.00030169	56	28	0.11003	-0.83024	
0.01552			8 S	-0.33605614	56	29	-0.00089	-0.44232	
0.01543			X	-0.48355040	56	30	0.00008	-0.43972	
0.00331			Y	-0.32569042	56	31	-0.00696	0.09421	-
0.00529			Z	0.00025284	56	32	-0.07991	-0.15083	
0.00009			9 S	0.00265793	56	33	-0.00032	-0.00257	
0.00008			X	-0.00452679	56	34	0.00201	-0.00230	
0.00006			Y	-0.00661426	56	35	0.00053	0.00161	-

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

0.00002		Z	0.00000379	56	36	0.00589	-0.00049	
0.00000		10	S	0.00101995	56	37	0.00005	-0.00001
0.00000		X	-0.00025365	56	38	-0.00017	0.00000	
0.00000		Y	-0.00224120	56	39	0.00006	0.00001	
0.00000		Z	0.00000007	56	40	-0.00362	0.00000	
0.00502		11	S	-0.00080471	56	41	0.01391	-0.14312
0.00203		X	-0.00048591	56	42	-0.00035	0.05799	-
0.00486		Y	0.00506666	56	43	-0.00842	0.13861	-
0.00146		Z	0.00000520	56	44	0.00284	-0.04173	
0.50777		12	S	0.04227011	56	45	0.49192	-7.48967
0.04396		X	-0.08364172	56	46	0.06537	-0.64844	
0.27695		Y	0.05823589	56	47	-0.50079	4.08506	-
0.39252		Z	0.00006273	56	48	0.69133	-5.78968	
0.00157		13	S	-0.01843081	56	49	0.00173	-0.01878
0.00000		14	S	0.00062841	56	50	-0.00017	-0.00002
0.00002		15	S	0.00261345	56	51	-0.00305	-0.00018
0.00012		16	S	0.00428496	56	52	0.00015	-0.00143
0.00193		17	S	-0.00048639	56	53	-0.01451	-0.02317
0.17773		18	S	0.03134345	56	54	-0.00228	-2.13281
0.17779		19	S	0.00573718	56	55	0.01355	-2.13354
1.00000		20	S	0.00573608	56	56	0.95536	0.00000
1	2,4,6-trihydroxyacetophenone		05-M					

DIPOLE MOMENT OF GROUND STATE IN DEBYE UNITS

		CONTRIBUTION	MOMENT	X	Y	Z		
		ATOMIC	6.16	5.19	3.32	0.00		
		POLARIZATION	1.42	1.39	0.27	0.00		
		TOTAL	7.50	6.58	3.59	0.00		
1	part	e ch	eton	ica	nari	ngin	a	05-M

SPECTROSCOPIC DATA FOR THE LOWEST 60 CONFIGURATIONS

TRANSITION		-----SINGLET-----					-----TRIPLET-----		
WAVELENGTH	SYMMETRY	ORBITAL	ENERGY	FREQUENCY	WAVELENGTH	OSCILLATOR	ENERGY	FREQUENCY	NM
			EV	CM-1	NM	STRENGTH	EV	CM-1	
1	A*	32 TO 33	4.329259	34919.01	286.377	0.4169	3.033182	24465.09	
408.75	2	AP	4.797456	38695.40	258.429	0.0001	4.797227	38693.55	
258.44	3	A*	4.847085	39095.70	255.783	0.8207	2.717010	21914.90	
456.31	4	A*	4.930220	39766.25	251.469	0.4363	3.724555	30041.57	
332.87	5	A*	5.383497	43422.30	230.296	0.5642	2.532689	20428.21	
489.52	6	AP	5.942370	47930.07	208.637	0.0000	5.941828	47925.70	
208.66	7	AP	6.118803	49353.14	202.621	0.0002	6.118803	49353.14	
202.62	8	A*	6.159176	49678.79	201.293	0.1002	5.337611	43052.20	
232.28	9	AP	6.279326	50647.89	197.442	0.0006	6.279320	50647.84	
197.44	10	A*	6.341495	51149.33	195.506	0.0048	5.113478	41244.38	
242.46									

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

11	AP	30 TO 34	6.447694	52005.92	192.286	0.0002	6.447691	52005.89
192.29								
12	A*	32 TO 36	6.920579	55820.12	179.147	0.0146	5.713008	46080.07
217.01								
13	A*	29 TO 33	6.949726	56055.22	178.396	0.0606	5.669143	45726.27
218.69								
14	AP	28 TO 33	6.967631	56199.63	177.937	0.0001	6.965681	56183.91
177.99								
15	A*	31 TO 36	7.155535	57715.24	173.264	0.0217	5.690336	45897.21
217.88								
16	AP	32 TO 39	7.250767	58483.36	170.989	0.0023	7.250767	58483.36
170.99								
17	AP	26 TO 33	7.301796	58894.95	169.794	0.0003	7.301783	58894.84
169.79								
18	AP	32 TO 38	7.460959	60178.73	166.172	0.0009	7.460958	60178.73
166.17								
19	AP	31 TO 38	7.487802	60395.24	165.576	0.0043	7.487782	60395.07
165.58								
20	A*	29 TO 34	7.508856	60565.06	165.112	0.0049	6.722581	54223.11
184.42								
21	AP	26 TO 34	7.615602	61426.05	162.797	0.0045	7.615602	61426.05
162.80								
22	AP	30 TO 36	7.624974	61501.64	162.597	0.0017	7.624738	61499.74
162.60								
23	A*	27 TO 33	7.727010	62324.64	160.450	0.0471	6.523228	52615.16
190.06								
24	AP	28 TO 34	7.806390	62964.91	158.819	0.0001	7.806366	62964.72
158.82								
25	AP	31 TO 39	7.911115	63809.60	156.716	0.0000	7.911111	63809.57
156.72								
26	A*	27 TO 34	8.258310	66610.02	150.128	0.0517	7.547763	60878.88
164.26								
27	AP	25 TO 33	8.570219	69125.82	144.664	0.0004	8.569063	69116.49
144.68								
28	AP	24 TO 33	8.776193	70787.16	141.269	0.0015	8.775866	70784.52
141.27								
29	AP	28 TO 35	8.814650	71097.35	140.652	0.0003	8.810030	71060.09
140.73								
30	A*	29 TO 35	8.835386	71264.61	140.322	0.1748	7.143992	57622.13
173.54								
31	A*	30 TO 37	8.922695	71968.83	138.949	0.0658	8.796597	70951.73
140.94								
32	AP	25 TO 34	9.186486	74096.52	134.959	0.0000	9.186472	74096.40
134.96								
33	AP	24 TO 34	9.305879	75059.52	133.228	0.0001	9.305874	75059.48
133.23								
34	AP	26 TO 35	9.466041	76351.35	130.973	0.0001	9.466008	76351.09
130.97								
35	AP	29 TO 37	9.487492	76524.37	130.677	0.0005	9.487157	76521.67
130.68								
36	A*	29 TO 36	9.488561	76532.99	130.663	0.0511	8.612407	69466.09
143.96								
37	A*	27 TO 35	9.503002	76649.48	130.464	0.1027	8.329649	67185.42
148.84								
38	AP	31 TO 40	9.735225	78522.54	127.352	0.0010	9.734896	78519.88
127.36								
39	AP	28 TO 36	9.787615	78945.11	126.670	0.0008	9.785608	78928.92
126.70								
40	AP	32 TO 40	9.912228	79950.21	125.078	0.0002	9.912215	79950.11
125.08								
41	AP	27 TO 37	10.084038	81336.00	122.947	0.0000	10.083265	81329.77
122.96								
42	AP	26 TO 36	10.190188	82192.20	121.666	0.0005	10.190174	82192.08
121.67								
43	AP	32 TO 42	10.227590	82493.87	121.221	0.0524	10.227583	82493.81
121.22								
44	A*	23 TO 33	10.249430	82670.02	120.963	0.0112	10.016175	80788.63
123.78								
45	A*	27 TO 36	10.291970	83013.15	120.463	0.0306	9.292003	74947.59
133.43								
46	AP	22 TO 33	10.300465	83081.66	120.364	0.0018	10.298775	83068.03
120.38								
47	A*	30 TO 38	10.330048	83320.27	120.019	0.0130	10.186990	82166.39
121.70								
48	AP	20 TO 33	10.391916	83819.30	119.304	0.0004	10.391241	83813.85
119.31								
49	AP	32 TO 43	10.405035	83925.11	119.154	0.0056	10.405031	83925.08
119.15								
50	A*	28 TO 37	10.455983	84336.05	118.573	0.0695	10.323551	83267.88
120.09								
51	AP	32 TO 41	10.533595	84962.05	117.700	0.0038	10.533589	84962.00
117.70								
52	AP	31 TO 41	10.545697	85059.66	117.565	0.0052	10.545545	85058.43
117.57								
53	AP	31 TO 42	10.573206	85281.55	117.259	0.0093	10.573040	85280.20
117.26								
54	AP	25 TO 35	10.604918	85537.33	116.908	0.0000	10.602180	85515.24
116.94								
55	AP	29 TO 38	10.656019	85949.50	116.347	0.0004	10.654924	85940.67
116.36								

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

56	A*	30 TO 40	10.685675	86188.70	116.024	0.0278	10.368684	83631.91	
119.57									
57	AP	24 TO 35	10.761888	86803.41	115.203	0.0033	10.761114	86797.18	
115.21									
58	A*	23 TO 34	10.769499	86864.80	115.121	0.0087	10.276518	82888.51	
120.64									
59	A*	30 TO 39	10.829787	87351.08	114.481	0.0189	10.791636	87043.36	
114.89									
60	AP	31 TO 43	10.898480	87905.15	113.759	0.0289	10.898392	87904.43	
113.76									
1		part	e ch	eton	ica	nari	ngin	a	05-M

SINGLET STATES AND SJ FROM S0 TRANSITIONS AFTER CONFIGURATION INTERACTION  
 FOR STATES OF LESS THAN 9.0 EV

CI COMPONENTS STATE	TRANS. SYMM.	ENERGY STATE EV	FREQUENCY CM-1	WAVELENGTH NM	OSCILLATOR STRENGTH	POLARIZATION			DIPOLE MOMENT
						X	Y	Z	
1	AP	3.3059	26664.83	375.026	0.000002				
2	A*	3.6747	29639.74	337.385	0.028602	0.905428	-0.424500	0.000169	
3	A*	4.6075	37162.86	269.086	0.319037	-0.139291	-0.990252	0.000122	
4	A*	5.3692	43307.16	230.909	0.738959	-0.476817	0.879002	-0.000103	
5	A*	5.4772	44178.45	226.355	0.967234	-0.775611	-0.631211	-0.000023	
6	AP	5.9846	48271.01	207.164	0.000351	-0.000422	-0.004213	0.999991	
7	AP	6.0026	48415.84	206.544	0.000337	0.006894	0.001584	0.999975	
8	AP	6.0563	48849.23	204.712	0.001040	0.000519	-0.001477	0.999999	
9	AP	6.1987	49997.43	200.010	0.000097				
10	A*	6.2220	50185.47	199.261	0.276232	0.920936	-0.389715	0.000007	
11	AP	6.3059	50862.48	196.609	0.004235	-0.000863	0.000453	-1.000000	
12	A*	6.3161	50944.72	196.291	0.096643	0.538363	0.842713	0.000076	
13	AP	6.7860	54734.33	182.701	0.000005				
14	A*	6.8116	54941.03	182.013	0.064947	-0.764042	0.645167	0.000327	
15	A*	6.8831	55518.15	180.121	0.032643	-0.985544	-0.169421	-0.000131	
16	AP	6.9554	56100.93	178.250	0.000240	-0.001147	-0.001970	-0.999997	
17	A*	7.0535	56892.25	175.771	0.027247	0.772276	-0.635287	-0.000376	
18	AP	7.3007	58886.25	169.819	0.000313	0.001435	0.002089	-0.999997	
19	AP	7.4483	60076.85	166.453	0.003523	0.003180	0.000243	0.999995	
20	A*	7.4871	60389.33	165.592	0.008882	0.877947	0.478757	-0.000563	
21	AP	7.5230	60679.50	164.800	0.000001				
22	AP	7.6911	62035.16	161.199	0.002446	0.005854	0.001336	-0.999982	
23	A*	7.8556	63362.10	157.823	0.126064	0.894273	0.447523	-0.000311	
24	AP	7.9289	63953.07	156.365	0.000041				
25	AP	7.9930	64469.74	155.112	0.000012				
26	A*	8.3266	67160.63	148.897	0.039557	0.999612	0.027865	-0.000072	
27	AP	8.4350	68035.10	146.983	0.001786	0.003264	0.000364	0.999995	
28	AP	8.5653	69085.88	144.747	0.000577	-0.001863	0.002668	0.999995	
29	A*	8.5990	69358.25	144.179	0.137012	0.214895	0.976637	-0.000216	
30	A*	8.7817	70831.44	141.180	0.124263	0.997994	0.063301	-0.000406	
31	AP	8.9140	71898.81	139.084	0.001163	-0.008945	0.002785	0.999956	
1		part	e ch	eton	ica	nari	ngin	a	05-M

CI COEFFICIENT MATRIX FOR SINGLET STATES OF SYMMETRY SPECIES A\*

CONFIGURATION	SCF STATE									
	2	3	4	5	10	12	14	15	17	20
23										
26										
1	0.79909	0.09347	-0.44088	-0.37637	0.07439	-0.03971	-0.06082	0.00064	-0.00591	0.03292
0.01686	0.01926									
3	-0.00901	0.90440	-0.08378	0.35197	0.06328	-0.18552	-0.04000	-0.00863	0.00484	-0.00728
0.02833	0.00013									
4	0.58068	-0.09831	0.57920	0.45707	-0.30489	-0.03529	0.06177	0.04995	-0.04063	-0.00207
0.02676	0.04931									
5	0.01979	-0.36697	-0.59061	0.68955	0.06797	-0.15115	-0.07636	0.00369	-0.01189	-0.02326
0.02507	0.02332									
8	0.13585	-0.04321	0.23526	0.15068	0.89165	0.25140	0.06278	-0.14932	0.04975	0.10518
0.03164	-0.00433									
10	-0.01883	-0.12195	0.18392	-0.14424	0.23513	-0.90902	-0.07309	0.03769	0.01375	-0.03529
0.10510	0.02248									
12	-0.01532	0.00460	0.01705	0.00545	0.12740	0.06597	-0.16805	0.94253	-0.05418	0.21131
0.08654	-0.05480									
13	-0.01218	0.00982	-0.10004	-0.01124	0.03436	-0.09519	0.81897	0.08604	-0.49288	0.09176
0.16601	0.00660									
15	0.02491	-0.01937	-0.04384	0.00712	0.00492	-0.07614	0.41432	0.12288	0.81075	-0.13459
0.31746	-0.03669									
20	-0.04368	-0.00999	-0.01777	0.00070	-0.10660	-0.07782	-0.02209	-0.17712	0.15096	0.91129
0.12515	0.27303									
23	-0.00048	0.04558	-0.02916	0.02224	-0.06644	0.05444	0.30397	0.13176	0.22008	0.11094
0.89160	-0.01012									
26	0.03380	-0.01392	0.00082	0.02642	-0.05285	-0.04553	-0.01412	-0.10920	0.01222	0.25019
0.02020	-0.95155									

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

30	-0.01518	-0.05198	0.05354	-0.00729	-0.00276	-0.03470	0.00236	-0.00374	-0.06407	0.06334
0.09976	-0.00295									
31	0.01019	0.03686	-0.06103	0.00507	-0.00380	0.05854	0.05524	0.00772	-0.00238	-0.00583
0.05769	0.03284									
36	0.00499	0.02133	-0.01295	0.00873	-0.03778	0.07036	-0.06268	-0.01104	0.08102	0.01703
0.06555	0.06029									
37	-0.00550	-0.03690	0.02329	-0.03529	0.04386	-0.07678	0.02703	-0.01791	-0.06570	-0.01232
0.00817	-0.00906									
44	-0.01289	0.00515	-0.00943	-0.02673	-0.00303	-0.00350	-0.00949	-0.01039	-0.00755	-0.02856
0.01210	0.04991									
45	-0.00019	0.01453	-0.00917	0.01689	0.00022	-0.00113	0.01310	0.01298	0.00681	-0.00320
0.07354	-0.04902									
47	-0.00405	-0.01110	-0.00357	0.03573	0.02912	-0.06116	-0.05515	-0.00831	-0.02796	0.01842
0.06696	-0.01227									
50	0.00909	0.02784	-0.05737	0.01999	0.01853	-0.00304	-0.01285	-0.00926	-0.00889	-0.00360
0.04648	0.02123									
56	-0.00553	-0.04780	0.01911	-0.02542	-0.01336	0.02452	-0.00010	0.01318	0.06971	-0.02226
0.08973	-0.00115									
58	-0.01537	-0.00878	0.00688	0.02114	0.02278	-0.00897	-0.02889	0.02913	0.00575	0.01205
0.02576	-0.03004									
59	0.00216	0.00515	-0.02352	-0.00160	0.03574	0.01272	-0.00716	0.01406	-0.00888	0.05624
0.01083	-0.02109									

	29	30
1	-0.01791	0.04157
3	-0.00344	0.04951
4	0.01490	-0.03092
5	0.00620	0.00358
8	0.00425	-0.01359
10	0.08555	-0.09450
12	-0.01205	-0.00634
13	-0.06608	-0.01182
15	-0.04637	0.10255
20	-0.01392	-0.02983
23	0.02906	-0.06832
26	0.02064	-0.04636
30	0.30640	0.89889
31	0.83936	-0.29592
36	-0.02649	-0.05851
37	-0.05036	0.06544
44	-0.05588	-0.04513
45	0.12831	0.21004
47	-0.36710	0.11630
50	0.07343	0.04873
56	0.12566	-0.01317
58	0.05938	0.04170
59	0.05701	-0.00960

1 part e ch eton ica nari ngin a 05-M

CI COEFFICIENT MATRIX FOR SINGLETs OF SYMMETRY SPECIES AP

CONFIGURATION	-----SCF STATE-----										
-----	1	6	7	8	9	11	13	16	18	19	
21	22										
	2	-0.72022	0.00007	0.56704	-0.00007	-0.18281	0.00022	-0.27649	0.10421	-0.00001	-0.04406
0.00002	0.00422										
	6	0.60975	0.00005	0.42739	-0.00005	-0.13180	0.00017	-0.27551	0.08884	-0.00001	-0.12465
0.00000	-0.02740										
	7	0.00000	0.86305	-0.00014	-0.44791	0.00000	-0.02685	0.00001	0.00000	-0.18640	0.00000
0.03186	0.00000										
	9	0.00000	0.45271	0.00001	0.84073	0.00003	0.16650	0.00004	-0.00001	0.09086	0.00000
0.09452	0.00007										
	11	0.06242	-0.00003	-0.25674	0.00003	-0.86968	0.00010	-0.15285	0.12251	-0.00002	0.16095
0.00011	0.24629										
	14	0.03209	0.00005	0.38771	-0.00001	-0.21798	-0.00024	0.74045	-0.27065	0.00003	-0.06112
0.00001	0.26146										
	16	-0.00001	-0.01194	0.00009	0.03813	-0.00007	-0.65741	-0.00032	0.00009	0.06169	-0.00001
0.65560	0.00014										
	17	-0.03867	-0.00001	-0.08269	0.00001	-0.05974	0.00005	-0.28968	-0.83598	0.00001	0.07066
0.00003	0.00577										
	18	0.00000	0.11993	-0.00005	-0.18278	0.00001	0.08496	0.00001	0.00001	0.88656	0.00000
0.01523	0.00008										
	19	0.00002	-0.10219	-0.00008	-0.11912	0.00006	0.54278	0.00016	-0.00003	-0.04867	0.00000
0.72457	0.00034										
	21	-0.00240	0.00001	0.10260	-0.00001	0.02213	-0.00001	0.10182	-0.04824	0.00002	0.86547
0.00012	-0.33558										
	22	-0.28526	-0.00005	-0.44284	0.00005	-0.00627	-0.00014	0.19147	-0.00255	0.00000	-0.07343
0.00002	0.13094										
	24	-0.00473	0.00000	-0.02874	0.00001	-0.24942	0.00002	0.09916	-0.19921	0.00004	-0.40645
0.00020	-0.66242										
	25	0.00000	-0.06309	0.00000	0.04025	0.00001	0.14257	0.00009	-0.00003	-0.31863	0.00000
0.06634	0.00004										
	27	0.04743	0.00001	0.07621	0.00000	0.09171	-0.00002	-0.21524	-0.08791	-0.00004	0.00667
0.00018	0.29597										

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

28	0.06350	0.00003	0.20928	-0.00002	-0.07894	0.00005	0.02666	-0.05561	0.00001	0.07801
0.00003	0.02511									
29	-0.04541	-0.00001	-0.04799	-0.00002	0.00879	0.00017	-0.11039	0.25046	0.00002	-0.03703
0.00013	-0.21154									
32	0.00130	-0.00001	-0.06535	0.00001	-0.04355	0.00000	-0.00866	0.09573	0.00000	0.08323
0.00001	0.06721									
33	-0.00981	-0.00001	-0.05030	0.00001	-0.20417	0.00003	0.00101	-0.03350	0.00001	0.03534
0.00009	-0.28972									
34	0.03239	0.00000	-0.00456	0.00000	0.09985	0.00002	-0.22371	-0.17047	-0.00002	0.00610
0.00008	0.14788									
35	0.00003	-0.00371	0.00002	0.07381	-0.00003	-0.31689	-0.00028	0.00009	-0.00698	-0.00001
0.03706	-0.00029									
38	-0.00002	-0.02588	0.00000	-0.06602	0.00001	0.10375	0.00012	-0.00004	-0.01711	0.00000
0.08771	0.00013									
39	0.02696	0.00000	-0.04808	0.00001	0.00158	-0.00008	0.02444	0.06152	-0.00002	-0.01226
0.00008	0.12121									
40	0.00000	-0.05356	0.00000	0.01636	0.00001	0.05656	0.00004	-0.00001	0.23028	0.00000
0.06500	0.00002									
41	-0.00005	0.06712	0.00008	0.14878	-0.00004	-0.26616	0.00007	-0.00003	0.00070	0.00000
0.01377	0.00019									
42	-0.01937	0.00000	0.00892	0.00000	0.09936	0.00000	-0.08021	-0.06489	-0.00001	-0.00719
0.00008	0.19107									
43	0.00000	-0.06241	0.00001	0.00119	0.00000	-0.01929	-0.00001	0.00000	0.02879	0.00000
0.03406	-0.00001									
46	-0.00737	0.00000	0.00422	0.00001	-0.01821	-0.00005	0.02658	0.01291	-0.00001	0.01312
0.00004	0.04430									
48	0.00196	0.00000	-0.04211	0.00001	0.00639	-0.00001	-0.03181	0.03806	0.00000	-0.00241
0.00001	-0.06657									
49	0.00000	0.00610	0.00000	0.01889	0.00000	0.01864	0.00001	0.00000	-0.06089	0.00000
0.00586	0.00000									
51	0.00000	-0.00750	0.00001	-0.02318	0.00000	-0.02173	0.00001	-0.00001	-0.06167	0.00000
0.02962	0.00004									
52	-0.00002	-0.02945	0.00002	-0.01193	-0.00001	-0.00869	0.00007	-0.00003	0.01329	0.00000
0.04036	0.00012									
53	0.00002	-0.00399	-0.00002	0.03672	0.00001	0.02866	-0.00008	0.00003	-0.01085	0.00000
0.04423	-0.00010									
54	-0.05870	-0.00001	-0.04510	0.00000	-0.01234	0.00008	-0.13096	-0.17165	0.00001	-0.05171
0.00001	0.02432									
55	-0.00006	-0.08721	0.00007	-0.08374	-0.00003	-0.17289	0.00015	-0.00006	-0.02613	0.00001
0.06904	0.00024									
57	-0.08701	0.00000	-0.01788	0.00000	-0.01899	-0.00001	0.00122	0.01178	0.00000	-0.09743
0.00000	0.01168									
60	-0.00001	0.02686	0.00001	0.01627	0.00000	-0.00280	0.00003	-0.00001	0.02516	0.00000
0.08183	0.00008									

	24	25	27	28	31
2	-0.05499	-0.00002	0.05802	-0.12263	0.01697
6	-0.21909	-0.00005	-0.06575	-0.48000	0.05987
7	0.00000	-0.01497	0.00000	0.00000	0.00000
9	0.00003	-0.01025	0.00005	-0.00003	-0.00002
11	0.11314	0.00004	-0.00743	0.12462	0.04798
14	0.00080	0.00004	-0.17079	0.00673	0.21433
16	0.00004	-0.18223	-0.00004	0.00002	0.00002
17	-0.35768	-0.00006	-0.03711	0.05309	0.04094
18	0.00008	-0.31262	0.00002	-0.00001	-0.00001
19	0.00010	0.06281	0.00013	-0.00006	-0.00005
21	0.14636	0.00001	-0.03675	-0.23073	0.08368
22	-0.11029	-0.00001	-0.29155	-0.68220	-0.17001
24	0.38050	0.00003	0.01958	-0.14306	0.01735
25	0.00017	-0.92282	-0.00003	0.00001	0.00001
27	0.59469	0.00012	-0.13822	-0.21547	-0.03279
28	-0.04366	0.00001	-0.36939	0.12082	-0.78662
29	-0.22270	-0.00002	-0.65260	0.17785	0.23318
32	-0.23488	-0.00004	0.03547	-0.18100	0.29848
33	-0.04978	-0.00003	0.09905	-0.05176	-0.17575
34	0.27605	0.00007	-0.29894	0.06108	0.09937
35	-0.00019	-0.01322	-0.00042	0.00023	0.00022
38	0.00006	0.06057	0.00007	-0.00002	0.00008
39	-0.14530	-0.00004	0.33155	-0.17859	-0.23857
40	0.00002	-0.03015	0.00002	-0.00001	0.00002
41	0.00013	0.00990	0.00032	-0.00017	-0.00015
42	0.23141	0.00006	0.02799	-0.06915	0.11165
43	0.00000	-0.02474	0.00001	-0.00001	-0.00001
46	-0.03867	-0.00002	0.15385	0.04440	-0.09973
48	0.03398	0.00000	-0.21210	0.07738	0.04998
49	0.00001	-0.06576	-0.00001	0.00000	0.00000
51	0.00002	-0.01601	0.00006	-0.00003	-0.00004
52	0.00008	-0.00314	0.00018	-0.00010	-0.00012
53	-0.00008	0.05500	-0.00018	0.00010	0.00011
54	0.04036	0.00002	0.03861	-0.10685	0.09531
55	0.00017	0.01033	0.00042	-0.00023	-0.00022
57	-0.10923	-0.00002	-0.11063	-0.09579	0.12260
60	0.00004	0.00282	0.00007	-0.00004	-0.00003

1 part e ch eton ica nari ngin a 05-M

ELECTRON DENSITIES FOR EXCITED SINGLETs

ATOM

STATE



Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

	1	2	3	4	5	6	7	8	9	10	11
12											
0											
	1	4.11005	3.94769	3.97321	3.98847	3.98022	3.91990	4.10517	3.96642	4.17283	3.96597
4.02374		4.01610									
	2	3.87370	3.82860	3.90260	3.90744	3.90253	3.77708	3.90942	3.88699	4.05718	3.68923
3.83344		3.82748									
	3	4.05661	4.00950	3.87108	3.92103	3.93466	4.14129	4.08197	3.98075	3.96120	3.98700
4.01226		3.76772									
	4	3.95940	3.92133	3.95163	3.93409	3.93896	3.88330	3.98228	3.91401	4.06723	3.75437
3.87054		3.78935									
	5	4.10225	3.94949	4.02020	4.05865	4.04438	3.93173	4.10466	4.06923	4.28174	3.91570
4.03606		4.08646									
	6	4.06825	3.96855	3.87578	3.84579	3.85673	3.88369	4.03587	3.77115	3.88866	4.00113
3.88401		3.84087									
	7	3.84628	3.76994	3.81945	3.76746	3.75654	3.77034	3.79939	3.76850	3.64515	4.02725
3.73121		4.06223									
	8	5.97924	6.50984	6.48216	6.48631	6.49386	6.48470	6.07755	6.43243	5.99849	6.57317
6.40654		6.51402									
	9	6.27913	6.29836	6.31641	6.30304	6.30090	6.31073	6.28818	6.32955	6.29234	6.28606
6.30849		6.31387									
	10	6.30470	6.29460	6.27819	6.28835	6.28986	6.30936	6.29963	6.29201	6.29479	6.29815
6.29749		6.27380									
	11	6.29784	6.28618	6.29093	6.28587	6.28640	6.31138	6.25888	6.31397	6.27287	6.27892
6.29681		6.28414									
	12	3.99483	4.07575	4.07624	4.07430	4.07548	4.09092	3.96858	4.09076	3.97628	4.07560
4.09124		4.07542									
	13	0.78422	0.78535	0.78534	0.78534	0.78535	0.78549	0.78429	0.78550	0.78426	0.78535
0.78602		0.78534									
	14	0.81277	0.81292	0.81293	0.81293	0.81293	0.81333	0.81253	0.81333	0.81256	0.81293
0.81375		0.81293									
	15	0.93912	0.94301	0.94303	0.94310	0.94302	0.96039	0.93582	0.96037	0.93567	0.94308
0.97648		0.94311									
	16	0.95765	0.95986	0.95992	0.96003	0.95990	0.98202	0.95512	0.98175	0.95445	0.95994
0.99179		0.96002									
	17	0.80936	0.80968	0.80967	0.80958	0.80968	0.81430	0.80270	0.81414	0.80457	0.80968
0.81242		0.80971									
	18	0.91139	0.91608	0.91613	0.91571	0.91607	0.91668	0.89294	0.91675	0.89809	0.91605
0.91757		0.91610									
	19	0.95661	0.95665	0.95756	0.95626	0.95628	0.95668	0.95251	0.95620	0.95082	0.96023
0.95508		0.96066									
	20	0.95661	0.95664	0.95755	0.95626	0.95628	0.95668	0.95253	0.95619	0.95084	0.96022
0.95506		0.96065									
	21										
	22										
24											
0											
	1	4.07221	4.00671	3.93242	4.00078	4.00797	3.94514	4.09403	4.10733	4.01623	4.13099
4.04129		4.05413									
	2	3.89488	3.90273	3.77601	3.87820	3.94613	3.70082	4.05200	4.05457	3.82511	4.01892
3.89145		3.90281									
	3	4.09996	4.10645	4.18845	4.06993	3.98195	4.10982	3.93348	4.00352	3.94886	4.00196
4.00687		4.05080									
	4	3.97803	3.96042	3.83375	3.95204	3.91500	3.79634	4.02004	4.02585	3.84507	4.01833
3.95224		3.95993									
	5	4.04858	3.98550	3.86667	3.97963	4.06104	3.92300	4.20148	4.19026	4.05314	4.20047
4.02225		4.05775									
	6	4.04335	3.96336	3.93369	3.98150	3.81184	4.00475	3.77738	3.79480	3.87733	3.87692
4.02166		3.92633									
	7	3.81705	3.77664	3.87551	3.82888	3.83872	3.78847	3.68770	3.64421	3.75480	3.71686
3.75054		3.81781									
	8	6.40174	6.25356	6.51859	6.50536	6.36401	6.49942	6.43060	6.14735	6.45401	6.41827
6.35384		6.44990									
	9	6.30420	6.30260	6.28298	6.28665	6.31360	6.28795	6.29331	6.30700	6.31117	6.31104
6.26079		6.28850									
	10	6.29495	6.27255	6.29797	6.29404	6.26876	6.32841	6.28856	6.26448	6.30240	6.28029
6.28040		6.26087									
	11	6.15539	6.28246	6.27918	6.24538	6.28472	6.28459	6.24857	6.28315	6.29389	6.15342
6.26566		6.24012									
	12	3.90587	4.06085	4.07377	4.01403	4.07019	4.12304	4.01494	4.05809	4.10047	3.90714
4.04494		3.98474									
	13	0.78411	0.78534	0.78535	0.78403	0.78534	0.78605	0.78443	0.78535	0.78613	0.78374
0.78533		0.78002									
	14	0.81088	0.81293	0.81292	0.80913	0.81293	0.81355	0.80979	0.81293	0.81378	0.81022
0.81293		0.80373									
	15	0.92291	0.94309	0.94302	0.87898	0.94301	0.96452	0.87722	0.94317	0.97713	0.91910
0.94312		0.91467									
	16	0.94579	0.96000	0.95987	0.89521	0.95991	0.98609	0.89327	0.96000	0.99280	0.94034
0.96014		0.93105									
	17	0.78471	0.80970	0.80968	0.79698	0.80970	0.81388	0.79719	0.80969	0.81316	0.78417
0.80965		0.79811									
	18	0.84758	0.91605	0.91608	0.89257	0.91638	0.92102	0.89347	0.91610	0.91782	0.84476
0.91631		0.88429									
	19	0.94387	0.94955	0.95705	0.95334	0.95442	0.96159	0.95127	0.94610	0.95836	0.94150
0.94035		0.94721									
	20	0.94395	0.94952	0.95704	0.95336	0.95440	0.96159	0.95129	0.94607	0.95835	0.94158
0.94024		0.94724									
	21										
	22										
	23										
	24										
	25										
	26										
	27										
	28										
	29										
	30										
	31										
0											

Supplementary Material for Organic & Biomolecular Chemistry  
 This journal is © The Royal Society of Chemistry 2004

1	4.08009	4.15687	4.10101	4.12144	4.10945	4.08100	4.04226
2	3.93006	4.06793	3.86207	3.92059	3.90786	3.83629	3.87638
3	3.82151	3.86095	4.06437	4.07301	4.12582	4.04250	4.08355
4	3.89403	4.02096	3.89173	3.94441	3.98183	3.84569	3.94104
5	4.14429	4.25878	4.07858	4.13400	4.15571	4.05550	4.02905
6	3.75923	3.82871	4.01077	3.95341	3.95062	3.94780	4.02027
7	3.71436	3.60221	3.92513	3.83980	3.71971	3.96047	3.79763
8	6.42517	6.27499	6.46081	6.08821	5.94195	6.19382	6.44339
9	6.33222	6.25895	6.29959	6.28299	6.29089	6.29673	6.30530
10	6.27481	6.27176	6.28231	6.28996	6.31244	6.27197	6.25297
11	6.30589	6.26342	6.14433	6.27443	6.31616	6.28123	6.23312
12	4.08366	4.03805	3.90035	3.98602	4.02179	4.05359	3.96617
13	0.78620	0.78535	0.78343	0.78328	0.78461	0.78526	0.78307
14	0.81407	0.81293	0.81169	0.81082	0.81326	0.81296	0.81078
15	0.99258	0.94305	0.92263	0.93293	0.95494	0.94444	0.91909
16	1.00045	0.95991	0.94429	0.95121	0.97754	0.96199	0.92763
17	0.81169	0.80967	0.78413	0.80536	0.81293	0.81001	0.79860
18	0.91659	0.91603	0.84276	0.90118	0.91361	0.91548	0.86931
19	0.95657	0.93482	0.94496	0.95348	0.95445	0.95166	0.95019
20	0.95656	0.93470	0.94504	0.95349	0.95444	0.95163	0.95022

ELECTRON DENSITY DIFFERENCES FOR EXCITED SINGLET  
 FROM GROUND STATE

ATOM	STATE											
	1	2	3	4	5	6	7	8	9	10	11	
12												
0												
1	0.07125	-0.09111	-0.06559	-0.05033	-0.05858	-0.11889	0.06637	-0.07238	0.13403	-0.07282	-	
0.01505	-0.02270											
2	0.04748	0.00238	0.07638	0.08122	0.07631	-0.04914	0.08320	0.06077	0.23096	-0.13699		
0.00722	0.00126											
3	0.03979	-0.00732	-0.14573	-0.09578	-0.08216	0.12448	0.06516	-0.03607	-0.05561	-0.02981	-	
0.00456	-0.24909											
4	0.09893	0.06086	0.09115	0.07362	0.07849	0.02283	0.12180	0.05353	0.20676	-0.10610		
0.01007	-0.07112											
5	0.04010	-0.11266	-0.04194	-0.00350	-0.01777	-0.13042	0.04251	0.00708	0.21959	-0.14645	-	
0.02608	0.02431											
6	0.21398	0.11428	0.02151	-0.00848	0.00246	0.02942	0.18159	-0.08312	0.03439	0.14686		
0.02974	-0.01341											
7	0.14215	0.06580	0.11532	0.06333	0.05241	0.06621	0.09526	0.06436	-0.05898	0.32312		
0.02708	0.35810											
8	-0.52955	0.00105	-0.02663	-0.02248	-0.01492	-0.02409	-0.43124	-0.07635	-0.51029	0.06438	-	
0.10224	0.00524											
9	-0.04108	-0.02184	-0.00379	-0.01717	-0.01931	-0.00947	-0.03203	0.00935	-0.02786	-0.03414	-	
0.01171	-0.00633											
10	0.00560	-0.00449	-0.02090	-0.01074	-0.00924	0.01026	0.00053	-0.00708	-0.00431	-0.00094	-	
0.00161	-0.02529											
11	0.00165	-0.01001	-0.00526	-0.01032	-0.00979	0.01519	-0.03731	0.01778	-0.02332	-0.01726		
0.00062	-0.01205											
12	-0.08042	0.00050	0.00099	-0.00095	0.00023	0.01567	-0.10667	0.01551	-0.09897	0.00035		
0.01599	0.00017											
13	-0.00113	0.00000	0.00000	0.00000	0.00000	0.00014	-0.00105	0.00015	-0.00108	0.00000		
0.00067	-0.00001											
14	-0.00016	0.00000	0.00000	0.00000	0.00000	0.00041	-0.00040	0.00041	-0.00036	0.00000		
0.00083	0.00000											
15	-0.00388	0.00000	0.00002	0.00010	0.00002	0.01739	-0.00718	0.01737	-0.00733	0.00008		
0.03347	0.00011											
16	-0.00220	0.00000	0.00006	0.00017	0.00004	0.02216	-0.00473	0.02189	-0.00540	0.00008		
0.03194	0.00017											
17	-0.00033	0.00000	-0.00002	-0.00011	-0.00001	0.00462	-0.00699	0.00446	-0.00512	-0.00001		
0.00274	0.00003											
18	-0.00469	-0.00001	0.00005	-0.00038	-0.00001	0.00060	-0.02314	0.00066	-0.01799	-0.00004		
0.00149	0.00001											
19	0.00125	0.00128	0.00219	0.00089	0.00092	0.00132	-0.00286	0.00084	-0.00454	0.00486	-	
0.00029	0.00529											
20	0.00125	0.00128	0.00219	0.00089	0.00092	0.00132	-0.00283	0.00083	-0.00453	0.00486	-	
0.00030	0.00529											
13												
14												
15												
16												
17												
18												
19												
20												
21												
22												
23												
24												
0												
1	0.03341	-0.03209	-0.10638	-0.03802	-0.03083	-0.09366	0.05523	0.06854	-0.02257	0.09219		
0.00249	0.01534											
2	0.06866	0.07650	-0.05022	0.05198	0.11991	-0.12540	0.22578	0.22834	-0.00111	0.19270		
0.06523	0.07659											
3	0.08314	0.08964	0.17164	0.05312	-0.03486	0.09301	-0.08334	-0.01329	-0.06796	-0.01485	-	
0.00994	0.03399											
4	0.11755	0.09995	-0.02672	0.09157	0.05453	-0.06413	0.15957	0.16538	-0.01540	0.15786		
0.09177	0.09946											
5	-0.01357	-0.07665	-0.19548	-0.08252	-0.00111	-0.13915	0.13933	0.12812	-0.00901	0.13832	-	
0.03990	-0.00440											
6	0.18908	0.10909	0.07942	0.12723	-0.04243	0.15048	-0.07690	-0.05947	0.02306	0.02265		
0.16738	0.07206											
7	0.11292	0.07250	0.17138	0.12474	0.13459	0.08434	-0.01644	-0.05992	0.05067	0.01273		
0.04640	0.11367											
8	-0.10705	-0.25523	0.00980	-0.00343	-0.14477	-0.00936	-0.07818	-0.36144	-0.05478	-0.09051	-	
0.15494	-0.05888											

Supplementary Material for Organic & Biomolecular Chemistry  
This journal is © The Royal Society of Chemistry 2004

9	-0.01601	-0.01760	-0.03723	-0.03355	-0.00660	-0.03225	-0.02689	-0.01320	-0.00903	-0.00916	-
0.05941	-0.03171										
10	-0.00414	-0.02654	-0.00113	-0.00505	-0.03033	0.02931	-0.01054	-0.03462	0.00330	-0.01880	-
0.01869	-0.03822										
11	-0.14080	-0.01373	-0.01701	-0.05081	-0.01147	-0.01160	-0.04762	-0.01304	-0.00230	-0.14277	-
0.03053	-0.05607										
12	-0.16938	-0.01440	-0.00148	-0.06122	-0.00506	0.04779	-0.06031	-0.01716	0.02522	-0.16811	-
0.03031	-0.09051										
13	-0.00124	0.00000	0.00000	-0.00131	-0.00001	0.00070	-0.00092	0.00000	0.00078	-0.00160	-
0.00001	-0.00533										
14	-0.00204	0.00000	0.00000	-0.00379	0.00000	0.00062	-0.00314	0.00000	0.00086	-0.00270	-
0.00000	-0.00919										
15	-0.02009	0.00009	0.00001	-0.06403	0.00001	0.02151	-0.06578	0.00016	0.03413	-0.02391	-
0.00012	-0.02834										
16	-0.01406	0.00014	0.00001	-0.06465	0.00006	0.02623	-0.06658	0.00014	0.03294	-0.01952	-
0.00028	-0.02881										
17	-0.02498	0.00002	0.00000	-0.01271	0.00001	0.00420	-0.01249	0.00001	0.00348	-0.02551	-
0.00003	-0.01158										
18	-0.06850	-0.00004	0.00000	-0.02351	0.00029	0.00493	-0.02261	0.00002	0.00173	-0.07133	-
0.00023	-0.03180										
19	-0.01150	-0.00581	0.00169	-0.00203	-0.00094	0.00622	-0.00410	-0.00927	0.00299	-0.01387	-
0.01502	-0.00816										
20	-0.01141	-0.00584	0.00168	-0.00200	-0.00096	0.00623	-0.00407	-0.00929	0.00299	-0.01378	-
0.01512	-0.00812										

	25	26	27	28	29	30	31
0							
1	0.04130	0.11807	0.06221	0.08264	0.07065	0.04220	0.00346
2	0.10384	0.24171	0.03585	0.09437	0.08164	0.01007	0.05016
3	-0.19530	-0.15587	0.04756	0.05619	0.10900	0.02569	0.06673
4	0.03356	0.16049	0.03126	0.08393	0.12136	-0.01479	0.08057
5	0.08214	0.19663	0.01644	0.07185	0.09356	-0.00665	-0.03309
6	-0.09504	-0.02557	0.15650	0.09914	0.09635	0.09353	0.16600
7	0.01022	-0.10192	0.22100	0.13567	0.01558	0.25634	0.09350
8	-0.08361	-0.23379	-0.04797	-0.42058	-0.56683	-0.31496	-0.06540
9	0.01201	-0.06125	-0.02061	-0.03722	-0.02931	-0.02347	-0.01491
10	-0.02429	-0.02734	-0.01678	-0.00914	0.01334	-0.02713	-0.04613
11	0.00970	-0.03277	-0.15185	-0.02176	0.01997	-0.01496	-0.06307
12	0.00841	-0.03720	-0.17490	-0.08923	-0.05346	-0.02166	-0.10908
13	0.00085	0.00000	-0.00192	-0.00207	-0.00073	-0.00009	-0.00228
14	0.00114	0.00000	-0.00123	-0.00211	0.00033	0.00004	-0.00214
15	0.04958	0.00004	-0.02038	-0.01007	0.01193	0.00143	-0.02391
16	0.04059	0.00005	-0.01557	-0.00864	0.01768	0.00213	-0.03222
17	0.00200	-0.00001	-0.02556	-0.00432	0.00324	0.00032	-0.01109
18	0.00050	-0.00006	-0.07332	-0.01491	-0.00247	-0.00061	-0.04678
19	0.00120	-0.02054	-0.01040	-0.00189	-0.00092	-0.00370	-0.00517
20	0.00120	-0.02066	-0.01032	-0.00188	-0.00092	-0.00373	-0.00514