

Supplementary Information

Investigation of the Protolytic Equilibrium of a Highly Brønsted Acidic Ionic Liquid and Residual Water using Raman Spectroscopy

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S1. The stoichiometric determinations of [2-Sea][TfO]

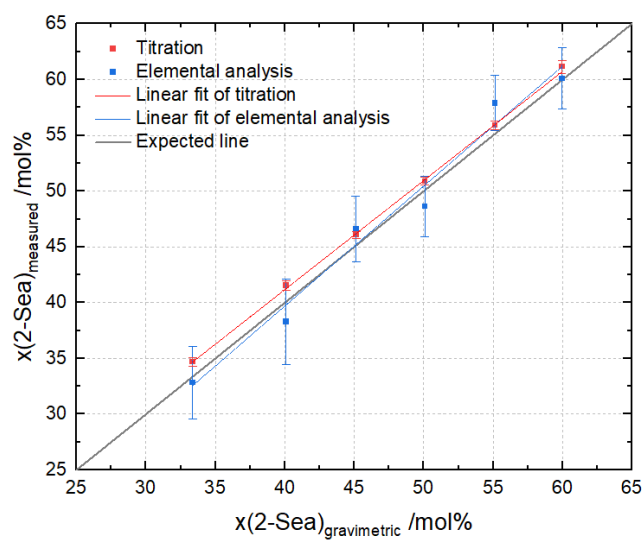
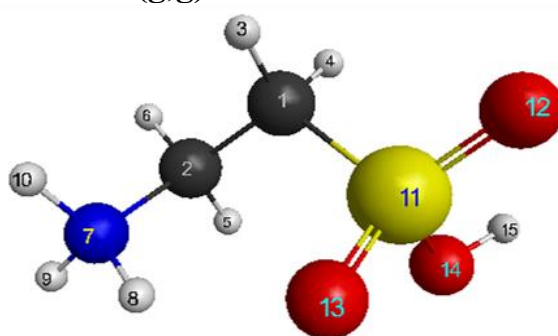


Fig. S1 The stoichiometric determinations on the series [2-Sea][TfO] compared to the initial weight.

S2. DFT calculations of 2-Sea⁺ (g,g)



NO.	TYPE	- - ATOMS - -						COORDINATE (BOHR, RAD)	COORDINATE (ANG, DEG)
		I	J	K	L	M	N		
1	STRETCH	2	1					2.8760468	1.5219385
2	STRETCH	3	1					2.0623660	1.0913572
3	STRETCH	4	1					2.0576177	1.0888445
4	STRETCH	5	2					2.0527901	1.0862898
5	STRETCH	6	2					2.0527123	1.0862487
6	STRETCH	7	2					2.8438783	1.5049157
7	STRETCH	8	7					1.9404366	1.0268349
8	STRETCH	9	7					1.9306153	1.0216377
9	STRETCH	10	7					1.9306596	1.0216611
10	STRETCH	11	1					3.3846021	1.7910544
11	STRETCH	12	11					2.7071799	1.4325780
12	STRETCH	13	11					2.7242144	1.4415923
13	STRETCH	14	11					3.0034207	1.5893419
14	STRETCH	15	14					1.8366717	0.9719249
15	BEND	11	1	2				1.9985428	114.5080650
16	BEND	3	1	2				1.9619284	112.4102190
17	BEND	4	1	2				1.9131714	109.6166486
18	TORSION	3	1	2	11			-2.0915783	-119.8386113
19	TORSION	4	1	2	11			2.0952406	120.0484424
20	BEND	7	2	1				1.9644468	112.5545099
21	BEND	5	2	1				1.9524719	111.8683985
22	BEND	6	2	1				1.9047249	109.1326995
23	TORSION	5	2	1	7			-2.1061752	-120.6749478
24	TORSION	6	2	1	7			2.0822724	119.3054189
25	BEND	8	7	2				1.9151343	109.7291141
26	BEND	9	7	2				1.9244285	110.2616328
27	BEND	10	7	2				1.9686945	112.7978864
28	TORSION	9	7	2	8			-2.1111970	-120.9626805
29	TORSION	10	7	2	8			2.0794561	119.1440555
30	BEND	12	11	1				1.9075357	109.2937441
31	BEND	13	11	1				1.8796309	107.6949201
32	BEND	14	11	1				1.8154653	104.0185000
33	TORSION	13	11	1	12			2.3094664	132.3226771
34	TORSION	14	11	1	12			-2.0398845	-116.8767703
35	BEND	15	14	11				1.9502338	111.7401636
36	TORSION	8	7	2	1			-0.9204675	-52.7389052
37	TORSION	11	1	2	7			1.1214534	64.2545444
38	TORSION	14	11	1	2			1.0834803	62.0788501
39	TORSION	15	14	11	1			1.6061545	92.0258742

TOTAL ENERGY DISTRIBUTION MATRIX M

(VIBR. CONTRIBUTIONS SUM TO 100 %)

			1	2	3	4
			0.29088E-04	0.14575E-04	0.13937E-04	0.22877E-04
			I	I	I	
STR.	2	1	0.00000000	0.00000000	0.00000000	0.00000000
STR.	3	1	0.00000000	0.00000000	0.00000000	0.00000000
STR.	4	1	0.00000000	0.00000000	0.00000000	0.00000000
STR.	5	2	0.00000000	0.00000000	0.00000000	0.00000000
STR.	6	2	0.00000000	0.00000000	0.00000000	0.00000000
STR.	7	2	0.00000000	0.00000000	0.00000000	0.00000000
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STR.	9	7	0.00000000	0.00000000	0.00000000	0.00000000
STR.	10	7	0.00000000	0.00000000	0.00000000	0.00000000
STR.	11	1	0.00000000	0.00000000	0.00000000	0.00000000
STR.	12	11	0.00000000	0.00000000	0.00000000	0.00000000
STR.	13	11	0.00000000	0.00000000	0.00000000	0.00000000
STR.	14	11	0.00000000	0.00000000	0.00000000	0.00000000
STR.	15	14	0.00000000	0.00000000	0.00000000	0.00000000
BEND	11	1 2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	3	1 2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	4	1 2	0.00000000	0.00000000	0.00000000	0.00000000
TORS	3	1 2 11	0.00000000	0.00000000	0.00000000	0.00000000
TORS	4	1 2 11	0.00000000	0.00000000	0.00000000	0.00000000
BEND	7	2 1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	5	2 1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	6	2 1	0.00000000	0.00000000	0.00000000	0.00000000
TORS	5	2 1 7	0.00000000	0.00000000	0.00000000	0.00000000
TORS	6	2 1 7	0.00000000	0.00000000	0.00000000	0.00000000
BEND	8	7 2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	9	7 2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	10	7 2	0.00000000	0.00000000	0.00000000	0.00000000
TORS	9	7 2 8	0.00000000	0.00000000	0.00000000	0.00000000
TORS	10	7 2 8	0.00000000	0.00000000	0.00000000	0.00000000
BEND	12	11 1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	13	11 1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	14	11 1	0.00000000	0.00000000	0.00000000	0.00000000
TORS	13	11 1 12	0.00000000	0.00000000	0.00000000	0.00000000
TORS	14	11 1 12	0.00000000	0.00000000	0.00000000	0.00000000
BEND	15	14 11	0.00000000	0.00000000	0.00000000	0.00000000
TORS	8	7 2 1	0.00000000	0.00000000	0.00000000	0.00000000
TORS	11	1 2 7	0.00000000	0.00000000	0.00000000	0.00000000
TORS	14	11 1 2	0.00000000	0.00000000	0.00000000	0.00000000
TORS	15	14 11 1	0.00000000	0.00000000	0.00000000	0.00000000

			5	6	7	8
			0.26036E-04	0.32911E-04	117.36	207.14
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STR.	3	1	0.00000000	0.00000000	0.00002295	0.00000531
STR.	4	1	0.00000000	0.00000000	-0.00003231	-0.00004725
STR.	5	2	0.00000000	0.00000000	-0.00000640	0.00001208
STR.	6	2	0.00000000	0.00000000	0.00000115	0.00008097
STR.	7	2	0.00000000	0.00000000	-0.00131770	-0.00024375
STR.	8	7	0.00000000	0.00000000	0.00000254	0.00028095
STR.	9	7	0.00000000	0.00000000	-0.00010623	-0.00005037

STR.	10	7			0.00000000	0.00000000	0.00017782	-0.00003616
STR.	11	1			0.00000000	0.00000000	0.00128956	0.03019001
STR.	12	11			0.00000000	0.00000000	0.00004177	0.00016432
STR.	13	11			0.00000000	0.00000000	-0.00003722	-0.00040159
STR.	14	11			0.00000000	0.00000000	-0.00053296	0.00029729
STR.	15	14			0.00000000	0.00000000	0.00002895	0.00000532
BEND	11	1	2		0.00000000	0.00000000	0.01980610	0.48191817
BEND	3	1	2		0.00000000	0.00000000	-0.00099885	0.00004970
BEND	4	1	2		0.00000000	0.00000000	-0.00035905	-0.00042614
TORS	3	1	2	11	0.00000000	0.00000000	-0.00192890	-0.00181765
TORS	4	1	2	11	0.00000000	0.00000000	-0.00245333	0.00054205
BEND	7	2	1		0.00000000	0.00000000	-0.00665455	-0.00284481
BEND	5	2	1		0.00000000	0.00000000	-0.00073003	0.00023233
BEND	6	2	1		0.00000000	0.00000000	0.00007367	-0.00111625
TORS	5	2	1	7	0.00000000	0.00000000	-0.00043721	0.00022173
TORS	6	2	1	7	0.00000000	0.00000000	-0.00030977	-0.00003036
BEND	8	7	2		0.00000000	0.00000000	-0.00007158	-0.00103848
BEND	9	7	2		0.00000000	0.00000000	0.00021616	-0.00039337
BEND	10	7	2		0.00000000	0.00000000	-0.00065202	-0.00024847
TORS	9	7	2	8	0.00000000	0.00000000	0.00003526	-0.00152070
TORS	10	7	2	8	0.00000000	0.00000000	-0.00092956	-0.00223611
BEND	12	11	1		0.00000000	0.00000000	0.01354812	0.13163278
BEND	13	11	1		0.00000000	0.00000000	-0.00057282	0.08801878
BEND	14	11	1		0.00000000	0.00000000	0.06524954	0.06348772
TORS	13	11	1	12	0.00000000	0.00000000	-0.02608267	0.00062056
TORS	14	11	1	12	0.00000000	0.00000000	0.02025876	0.02249762
BEND	15	14	11		0.00000000	0.00000000	-0.00024686	0.00014006
TORS	8	7	2	1	0.00000000	0.00000000	-0.00055927	0.00140056
TORS	11	1	2	7	0.00000000	0.00000000	-0.09600558	0.16979916
TORS	14	11	1	2	0.00000000	0.00000000	1.02303786	0.02371176
TORS	15	14	11	1	0.00000000	0.00000000	-0.00298876	0.00450071

9	10	11	12
281.28	301.54	350.65	380.36

STR.	2	1			0.03930532	0.00673134	0.01042302	0.01670231
STR.	3	1			0.00000819	0.00011286	0.00000056	0.00027903
STR.	4	1			0.00001236	0.00000644	0.00000251	0.00010189
STR.	5	2			0.00000117	-0.00006518	-0.00000334	0.00000639
STR.	6	2			-0.00000507	-0.00004883	-0.00001689	0.00001127
STR.	7	2			0.00871550	0.00002894	0.00148434	0.00250237
STR.	8	7			0.00007931	0.00006630	0.00002053	-0.00001775
STR.	9	7			-0.00016347	0.00001527	-0.00000612	-0.00007411
STR.	10	7			-0.00002929	0.00008055	-0.00001431	0.00009313
STR.	11	1			0.01150552	0.00140157	0.00303436	0.06083564
STR.	12	11			0.00160600	0.00039495	-0.00035672	0.00011616
STR.	13	11			0.00025844	-0.00035688	0.00179314	-0.00002415
STR.	14	11			-0.00039614	-0.00070808	0.00040456	-0.00013285
STR.	15	14			-0.00006861	-0.00004093	-0.00004259	-0.00000471
BEND	11	1	2		0.01684557	0.01252239	-0.00269011	0.09811473
BEND	3	1	2		0.00000492	0.00038395	-0.00008145	0.00033378
BEND	4	1	2		0.00173873	0.00211203	0.00073407	0.00988178
TORS	3	1	2	11	0.00120581	0.01230040	0.00002387	0.01542829
TORS	4	1	2	11	0.00355107	0.01406755	0.00146416	0.01387873
BEND	7	2	1		0.21352252	-0.00079267	0.03739050	0.12797366
BEND	5	2	1		-0.00052416	0.00027764	0.00006807	-0.00698732
BEND	6	2	1		-0.00048147	-0.00121381	-0.00115512	-0.00055183
TORS	5	2	1	7	-0.00102108	-0.00464012	-0.00263579	-0.00503927
TORS	6	2	1	7	-0.00035670	-0.00275885	-0.00019114	-0.01237058

BEND	8	7	2		-0.00221118	-0.00148091	-0.00154678	-0.00151326
BEND	9	7	2		0.00060107	0.00061610	0.00001253	0.00242052
BEND	10	7	2		0.00073637	-0.00331073	0.00007237	-0.00559379
TORS	9	7	2	8	-0.00015750	-0.00057189	-0.00033446	0.00101551
TORS	10	7	2	8	-0.00168778	-0.00057496	-0.00074723	0.00078722
BEND	12	11	1		0.21195540	0.08642798	0.07831266	0.02248521
BEND	13	11	1		0.25014450	0.08222320	0.02477515	0.07063404
BEND	14	11	1		0.05469463	0.56603633	-0.01255555	0.01168002
TORS	13	11	1	12	0.01104726	-0.02169667	0.00384359	0.01055726
TORS	14	11	1	12	0.01937200	0.00412447	0.07462220	-0.00007906
BEND	15	14	11		0.00035617	0.00009379	-0.00022938	0.00002646
TORS	8	7	2	1	0.00088329	0.00002644	-0.00165623	-0.00159483
TORS	11	1	2	7	0.02981608	0.14969472	0.08302562	0.67318089
TORS	14	11	1	2	0.00055494	0.08944476	-0.01610953	-0.12125353
TORS	15	14	11	1	0.12858032	0.00907054	0.71886493	0.01619079

13	14	15	16
438.53	459.28	483.59	575.90

STR.	2	1			0.00059466	0.00378098	0.00691878	0.00643448
STR.	3	1			0.00001469	0.00008078	-0.00001031	-0.00017020
STR.	4	1			0.00002673	0.00004250	0.00000736	0.00006694
STR.	5	2			-0.00000326	-0.00001747	-0.00000164	-0.00001742
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STR.	7	2			0.00835249	0.00348663	0.00028963	0.00221765
STR.	8	7			0.00003294	0.00001272	0.00000174	-0.00000276
STR.	9	7			-0.00017116	-0.00010608	-0.00000854	-0.00003062
STR.	10	7			-0.00003046	0.00002834	0.00000339	-0.00002119
STR.	11	1			0.03873700	0.10273181	0.10403508	0.00641659
STR.	12	11			0.00133057	0.00015914	0.00416358	0.01193973
STR.	13	11			0.00149032	0.00164866	-0.00002553	0.00082443
STR.	14	11			0.00189871	0.00507888	0.02249442	0.00220761
STR.	15	14			0.00009707	-0.00001908	0.00024955	0.00001547
BEND	11	1	2		0.00233809	0.02785951	-0.00062876	0.21746993
BEND	3	1	2		0.00522014	0.00937044	0.00026150	0.00867011
BEND	4	1	2		0.00241855	0.00231691	0.00011292	0.00063991
TORS	3	1	2	11	0.00180660	0.01880436	0.00884805	0.00321394
TORS	4	1	2	11	0.00305262	0.03605472	0.00027865	-0.00064812
BEND	7	2	1		0.23617518	0.13878251	0.00852950	0.06757877
BEND	5	2	1		0.00390939	0.00503624	0.00017746	0.01491640
BEND	6	2	1		0.00090788	0.00052327	-0.00114820	-0.00136956
TORS	5	2	1	7	-0.00236993	-0.00050282	0.00005832	0.00216348
TORS	6	2	1	7	0.00074028	0.00007938	-0.00020587	0.00759162
BEND	8	7	2		-0.00238456	-0.00051536	0.00002870	0.00095680
BEND	9	7	2		0.00428142	0.00506215	0.00079375	0.00599440
BEND	10	7	2		0.00160217	0.00101105	0.00002795	0.00129479
TORS	9	7	2	8	0.00103606	0.00168488	0.00017416	0.00179677
TORS	10	7	2	8	-0.00165282	-0.00070773	-0.00024462	-0.00050456
BEND	12	11	1		0.07534102	0.11667232	0.06914108	0.00460159
BEND	13	11	1		-0.00087410	-0.03694363	0.06462939	0.34503539
BEND	14	11	1		0.01719806	0.01373806	-0.00247073	0.15798005
TORS	13	11	1	12	-0.04366299	0.16081042	0.75598076	0.08511447
TORS	14	11	1	12	0.54627798	0.30772582	-0.06822580	0.00693175
BEND	15	14	11		0.02201557	0.01232793	0.00035548	0.00231388
TORS	8	7	2	1	0.00352216	0.00638220	0.00347906	-0.01016047
TORS	11	1	2	7	0.00932196	0.00364105	-0.00028585	0.04434910
TORS	14	11	1	2	-0.00963910	0.02356616	-0.00401955	0.00857338
TORS	15	14	11	1	0.07102803	0.03026475	0.02621997	-0.00450991

			17 713.15	18 820.98	19 829.94	20 849.08
STR.	2	1	0.00746069	0.00093844	0.08477606	0.06580064
STR.	3	1	-0.00023984	-0.00007799	-0.00003198	-0.00030477
STR.	4	1	-0.00003709	-0.00003682	0.00014101	0.00011097
STR.	5	2	0.00001589	-0.00000096	0.00002977	-0.00029380
STR.	6	2	-0.00000231	0.00000304	-0.00001259	-0.00000274
STR.	7	2	0.00073457	0.03985526	0.06388237	0.30010598
STR.	8	7	-0.00000756	0.00012655	0.00003485	-0.00009967
STR.	9	7	0.00000205	0.00009947	0.00043285	0.00005984
STR.	10	7	-0.00000011	-0.00020789	0.00025281	0.00011060
STR.	11	1	0.46250600	0.07346942	0.01446486	0.02861672
STR.	12	11	0.01217545	0.00006575	0.00254306	0.00083099
STR.	13	11	0.02108897	0.00155859	0.00033373	0.00054018
STR.	14	11	0.20206917	0.25896455	0.29148635	0.19892780
STR.	15	14	0.00015385	0.00002988	0.00002195	0.00000265
BEND	11	1 2	0.09739368	0.04702436	-0.03372123	-0.00189307
BEND	3	1 2	-0.00204762	0.01354691	0.00285873	0.01679010
BEND	4	1 2	0.00154614	0.02054267	0.00079614	0.09936024
TORS	3	1 2 11	0.00708503	0.04456558	0.00057145	0.06902896
TORS	4	1 2 11	-0.00719993	0.08254012	0.00193332	0.06828672
BEND	7	2 1	-0.00096266	-0.00251168	0.00981052	-0.00128024
BEND	5	2 1	0.00780431	0.00446218	0.00252041	0.02320498
BEND	6	2 1	0.00086551	0.00036437	0.00050425	0.00341307
TORS	5	2 1 7	0.00839458	0.00038440	0.00173163	0.02323884
TORS	6	2 1 7	0.00664408	0.00197585	0.00292162	0.01815261
BEND	8	7 2	-0.00003386	0.02007272	0.01043477	0.00022215
BEND	9	7 2	0.00013951	0.03757550	0.05827151	0.00043378
BEND	10	7 2	0.00000504	0.00345253	0.00023568	-0.00086234
TORS	9	7 2 8	-0.00003409	0.01378570	0.01451776	0.00011126
TORS	10	7 2 8	-0.00001211	0.00076287	-0.00327537	-0.00058034
BEND	12	11 1	0.11081703	0.01021452	0.04923550	-0.00000608
BEND	13	11 1	0.03853435	-0.00002965	-0.00010442	0.04565422
BEND	14	11 1	0.02146563	0.01865606	-0.00105572	-0.00356417
TORS	13	11 1 12	-0.00112749	-0.00490994	0.03439986	0.01570198
TORS	14	11 1 12	0.00340099	0.00036374	-0.00509227	0.00965113
BEND	15	14 11	-0.00169542	-0.00194358	-0.00156578	0.00578525
TORS	8	7 2 1	-0.00061621	0.31937632	0.40745817	0.01128756
TORS	11	1 2 7	0.00359537	-0.01344463	-0.01041615	0.00891947
TORS	14	11 1 2	0.00011044	0.00780226	-0.00175137	-0.00459201
TORS	15	14 11 1	0.00000795	0.00058353	0.00042588	-0.00086946

			21 950.23	22 981.77	23 1052.7	24 1123.0
STR.	2	1	0.17711048	0.06761798	0.34836807	0.05491513
STR.	3	1	-0.00038602	-0.00032184	0.00017983	0.00003660
STR.	4	1	-0.00025667	-0.00013181	-0.00004903	0.00000480
STR.	5	2	0.00017801	-0.00073127	-0.00009136	-0.00005421
STR.	6	2	-0.00005029	-0.00021863	0.00011927	-0.00001432
STR.	7	2	0.16429506	0.09091876	0.29415973	0.03079174
STR.	8	7	0.00023571	-0.00002519	-0.00013839	0.00005887
STR.	9	7	0.00006837	0.00000627	0.00010152	0.00039740
STR.	10	7	-0.00003173	0.00001229	-0.00013499	-0.00018142
STR.	11	1	0.02338897	0.01310750	0.00335716	-0.00000219
STR.	12	11	0.00066982	0.00083008	-0.00004026	0.00997688
STR.	13	11	0.00780278	0.00268280	0.00063523	0.00004071
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STR.	15	14		-0.00000013	-0.00000111	-0.00000050	-0.00010031
BEND	11	1	2	-0.00742815	0.00953790	0.02503135	-0.00527029
BEND	3	1	2	0.04000300	-0.00314601	0.01757937	0.07105570
BEND	4	1	2	-0.01195670	0.03193355	0.00033577	0.12547346
TORS	3	1	2 11	0.05447044	0.12806083	0.00455893	0.04439278
TORS	4	1	2 11	0.18662155	0.05116211	0.00074517	0.05905884
BEND	7	2	1	0.13625832	0.00389512	0.00875954	-0.00601824
BEND	5	2	1	0.01392429	0.03642093	0.01204431	0.12136324
BEND	6	2	1	0.02233442	0.04803006	-0.01127942	-0.00239159
TORS	5	2	1 7	0.01991459	0.25478847	0.03996167	-0.00441168
TORS	6	2	1 7	0.03064354	0.17653080	0.05965516	0.01517548
BEND	8	7	2	0.00059665	0.01944875	0.01566332	0.01163475
BEND	9	7	2	0.01360484	0.01855507	0.04643157	0.14448571
BEND	10	7	2	-0.00089604	0.02011926	0.05034218	0.04947004
TORS	9	7	2 8	-0.01595366	0.01702296	0.02074633	0.02520007
TORS	10	7	2 8	-0.00769341	-0.00249257	-0.01405889	-0.00744756
BEND	12	11	1	-0.00286739	0.00135708	0.00720873	0.00291791
BEND	13	11	1	0.00555001	0.00930382	0.00667386	-0.00004976
BEND	14	11	1	0.00673209	0.00757544	-0.00090081	0.00525923
TORS	13	11	1 12	-0.00178885	0.00624701	-0.00052261	0.00440083
TORS	14	11	1 12	0.00514753	0.00036561	-0.00052071	0.00456675
BEND	15	14	11	0.00333371	0.00132331	0.00538443	0.18594382
TORS	8	7	2 1	0.14680700	-0.00005008	0.05352927	0.07641640
TORS	11	1	2 7	0.00998843	-0.01540607	0.00202825	-0.01393457
TORS	14	11	1 2	-0.02007145	0.00114919	0.00431634	-0.00048344
TORS	15	14	11 1	0.00009534	0.00001222	-0.00018938	0.00045070

25	26	27	28
1131.2	1165.4	1251.4	1285.6

STR.	2	1		0.00884620	0.00163098	0.05225756	0.00518993
STR.	3	1		0.00000489	-0.00005852	0.00000398	-0.00001494
STR.	4	1		-0.00000044	-0.00002938	0.00001303	0.00001567
STR.	5	2		0.00000658	-0.00001706	0.00031238	0.00001602
STR.	6	2		-0.00000035	-0.00001533	0.00003315	0.00009850
STR.	7	2		0.00179253	0.00006113	0.00696051	-0.00008736
STR.	8	7		0.00004774	0.00000849	0.00000484	-0.00001282
STR.	9	7		0.00009720	0.00005039	0.00023839	0.00030945
STR.	10	7		-0.00004906	-0.00004682	-0.00034460	-0.00004266
STR.	11	1		0.00249837	0.00894602	0.00149574	0.00108204
STR.	12	11		0.01989941	0.37409649	0.02484638	0.01427076
STR.	13	11		0.25373173	0.31893552	0.00826886	0.07439163
STR.	14	11		-0.00747136	0.02368768	0.00185351	-0.00012150
STR.	15	14		-0.00030410	-0.00017440	-0.00000531	0.00001275
BEND	11	1	2	0.00051208	-0.00318034	0.00278268	-0.01939302
BEND	3	1	2	0.01814058	0.00354960	0.10223685	0.33848958
BEND	4	1	2	0.00289973	0.00525108	0.44442843	0.04463337
TORS	3	1	2 11	0.01905018	0.00119816	-0.00284026	0.17409618
TORS	4	1	2 11	0.00244259	0.03220897	0.04197096	0.09322881
BEND	7	2	1	0.00024986	0.00037310	0.04929957	0.00070319
BEND	5	2	1	0.02070583	0.01540550	0.05001274	0.01359602
BEND	6	2	1	-0.00018772	0.00145487	0.00225370	0.00461647
TORS	5	2	1 7	0.00080586	0.00227807	0.01635902	0.04702068
TORS	6	2	1 7	0.00028460	0.00086390	-0.00462598	0.05169047
BEND	8	7	2	0.00247121	0.00456887	0.03513421	0.01825983
BEND	9	7	2	0.02995409	0.01939713	0.05894240	0.09139871
BEND	10	7	2	0.01257276	0.00916276	0.04560925	-0.00053984
TORS	9	7	2 8	0.00981767	0.00508092	0.07182940	-0.00813339
TORS	10	7	2 8	-0.00154192	-0.00126908	-0.00001048	-0.00455638

BEND	12	11	1	0.00640161	0.00072495	0.00094433	0.00008064
BEND	13	11	1	0.00118581	-0.00021636	0.00036175	0.00082812
BEND	14	11	1	0.00009886	0.00680099	0.00007535	0.00218130
TORS	13	11	1 12	0.00038531	0.00892658	0.00001776	0.00103986
TORS	14	11	1 12	0.00938563	0.01724337	0.00011391	0.00034993
BEND	15	14	11	0.57432897	0.13701705	0.00232183	0.00311685
TORS	8	7	2 1	0.01177179	0.01060416	-0.00144028	0.05598062
TORS	11	1	2 7	-0.00212864	-0.00639459	-0.01467805	-0.00381886
TORS	14	11	1 2	0.00002396	0.00187549	0.00297423	0.00003862
TORS	15	14	11 1	0.00126994	-0.00000036	-0.00001173	-0.00001520

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1357.3	1397.6	1449.6	1467.5

STR.	2	1	0.00141582	0.01797714	0.00128846	0.00335943
STR.	3	1	0.00000386	-0.00000394	0.00003536	-0.00014855
STR.	4	1	-0.00000576	-0.00004512	0.00000810	-0.00041957
STR.	5	2	-0.00000413	0.00003324	-0.00004886	0.00000009
STR.	6	2	0.00000910	-0.00058001	0.00029609	-0.00000026
STR.	7	2	-0.00002666	0.00066759	0.00300469	0.00018133
STR.	8	7	0.00001768	-0.00038508	-0.00036789	-0.00000702
STR.	9	7	-0.00000221	0.00068839	0.00007416	0.00000327
STR.	10	7	-0.00000247	-0.00000144	-0.00005818	-0.00000130
STR.	11	1	0.00285375	0.00588912	-0.00096912	-0.00047741
STR.	12	11	0.51417761	0.00097986	0.00334520	0.00102181
STR.	13	11	0.28584575	0.01405615	0.00267047	0.00069771
STR.	14	11	-0.00119808	-0.00001692	-0.00002244	-0.00001134
STR.	15	14	-0.00004179	0.00000240	-0.00000011	-0.00000084
BEND	11	1 2	0.01063632	0.00876157	0.00820530	-0.00531498
BEND	3	1 2	0.01730970	0.03547550	0.04013003	0.25331314
BEND	4	1 2	0.04350740	0.01311916	0.00359762	0.15290067
TORS	3	1 2 11	0.00499281	0.07235969	-0.00059035	0.32183448
TORS	4	1 2 11	0.02489462	0.04360821	-0.00043927	0.25043828
BEND	7	2 1	0.00090403	-0.00409445	-0.00797757	0.00001573
BEND	5	2 1	0.00309736	0.21303956	0.37864536	0.00168062
BEND	6	2 1	-0.00011922	0.07964750	-0.00168993	0.00015504
TORS	5	2 1 7	0.00580297	0.00257313	0.19319461	0.00773878
TORS	6	2 1 7	0.00343913	0.05332415	0.02917779	0.00170447
BEND	8	7 2	0.00366353	0.18066061	0.20223059	0.00653697
BEND	9	7 2	0.00004586	0.20391568	0.02199915	0.00093864
BEND	10	7 2	0.00004032	0.02660629	0.04379697	0.00012154
TORS	9	7 2 8	-0.00001841	0.02461215	0.12166855	0.00370602
TORS	10	7 2 8	-0.00000919	-0.00669272	0.00430876	0.00004250
BEND	12	11 1	0.00144863	-0.00023541	-0.00039130	0.00065153
BEND	13	11 1	0.00482229	-0.00007366	0.00003127	-0.00010070
BEND	14	11 1	0.00091235	0.00042770	-0.00019843	0.00029287
TORS	13	11 1 12	0.00077012	0.00008329	-0.00009670	-0.00006972
TORS	14	11 1 12	0.02007650	0.00020890	0.00133473	-0.00000732
BEND	15	14 11	0.04870990	0.00047434	0.00019217	0.00034633
TORS	8	7 2 1	0.00002178	0.01498156	-0.03454413	-0.00023551
TORS	11	1 2 7	0.00058659	-0.00165998	-0.00529917	-0.00094056
TORS	14	11 1 2	0.00092212	-0.00041346	-0.00655126	-0.00036745
TORS	15	14 11 1	0.00050005	0.00002928	0.00000926	0.00042127

33	34	35	36
1542.0	1701.7	1726.0	1903.6

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STR.	5	2			0.00006326	0.00007659	0.00006918	0.00005814
STR.	6	2			0.00026816	0.00127585	-0.00000138	0.00006785
STR.	7	2			-0.00824918	-0.00385743	-0.00868947	-0.00078871
STR.	8	7			0.00016108	0.00020223	0.00011322	0.00076064
STR.	9	7			0.00010982	0.00003191	-0.00052949	-0.00084887
STR.	10	7			-0.00000189	-0.00001090	-0.00011732	0.00032796
STR.	11	1			0.00005942	-0.00036240	0.00005146	-0.00006266
STR.	12	11			0.00033844	0.00006954	0.00012309	0.00014473
STR.	13	11			0.00003737	0.00032052	0.00019944	0.00061932
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STR.	15	14			0.00000081	0.00000012	0.00000105	0.00000000
BEND	11	1	2		-0.00062829	-0.00760947	0.00011009	-0.00019461
BEND	3	1	2		0.01015197	0.00104123	0.00037696	0.00000569
BEND	4	1	2		0.00007863	0.00211534	0.00005142	0.00009159
TORS	3	1	2	11	0.00009315	0.00006325	0.00054223	-0.00000041
TORS	4	1	2	11	-0.00024882	-0.00004582	0.00012110	0.00001155
BEND	7	2	1		-0.00999897	0.00902135	-0.00297778	-0.00212271
BEND	5	2	1		-0.00141486	0.06649420	0.00092102	-0.00004002
BEND	6	2	1		0.00156192	0.84942852	0.00314102	0.00406206
TORS	5	2	1	7	0.37484188	0.01111923	0.00883406	0.00122930
TORS	6	2	1	7	0.55091888	0.00680131	0.00052683	0.00080057
BEND	8	7	2		0.02632559	0.01620423	0.13439535	0.15587121
BEND	9	7	2		0.03348542	0.02329786	0.05615462	0.11090037
BEND	10	7	2		0.01714846	0.00054700	0.67750800	0.02756474
TORS	9	7	2	8	0.00470600	0.00950585	0.10176524	0.37572510
TORS	10	7	2	8	-0.00077744	-0.00005428	0.02891887	0.38552455
BEND	12	11	1		0.00016572	0.00127516	-0.00006283	0.00003577
BEND	13	11	1		-0.00005561	0.00003722	0.00018683	0.00006819
BEND	14	11	1		0.00001181	-0.00001055	0.00003389	-0.00004296
TORS	13	11	1	12	0.00000949	0.00005838	0.00004407	-0.00007892
TORS	14	11	1	12	-0.00003591	0.00020054	-0.00042397	0.00025080
BEND	15	14	11		-0.00000180	0.00000440	-0.00000415	0.00001895
TORS	8	7	2	1	-0.00053900	-0.00044911	-0.00217259	-0.06045733
TORS	11	1	2	7	0.00241663	-0.00003674	-0.00113361	0.00052495
TORS	14	11	1	2	-0.00423181	-0.00028522	0.00183817	-0.00000517
TORS	15	14	11	1	0.00000565	-0.00000114	0.00000875	-0.00000629

37	38	39	40
1917.7	3082.9	3137.6	3144.0

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STR.	8	7			0.00056462	0.00000119	0.00036658	0.00046772
STR.	9	7			0.00000191	0.00000063	-0.00000052	-0.00000007
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STR.	11	1			0.00000695	-0.00012201	-0.00001905	0.00004069
STR.	12	11			0.00006327	0.00000342	-0.00000005	0.00000008
STR.	13	11			0.00025445	0.00000035	0.00000249	0.00000347
STR.	14	11			0.00001235	0.00000242	0.00000240	0.00000360
STR.	15	14			0.00000031	0.00000103	0.00000028	0.00000000
BEND	11	1	2		0.00018336	-0.00007614	0.00021352	0.00016658
BEND	3	1	2		0.00000581	0.00001219	-0.00010055	-0.00022568
BEND	4	1	2		-0.00000045	-0.00016517	0.00029926	-0.00002378
TORS	3	1	2	11	0.00000738	-0.00004710	-0.00091611	-0.00046857

TORS	4	1	2	11	0.00004736	-0.00082594	-0.00014246	-0.00019095
BEND	7	2	1		-0.00242779	-0.00000210	0.00115298	0.00000547
BEND	5	2	1		0.00004566	0.00007946	0.00008846	-0.00006595
BEND	6	2	1		-0.00000009	0.00006233	0.00004077	0.00021195
TORS	5	2	1	7	0.00006372	-0.00002943	-0.00013332	-0.00021692
TORS	6	2	1	7	-0.00018503	-0.00000084	-0.00031023	0.00049726
BEND	8	7	2		0.14581382	0.00000160	0.00010352	0.00014597
BEND	9	7	2		0.00767214	0.00000118	0.00012057	0.00006148
BEND	10	7	2		0.02230227	-0.00000175	0.00000305	-0.00000669
TORS	9	7	2	8	0.20184160	0.00000024	0.00000003	0.00000078
TORS	10	7	2	8	0.63990092	0.00000002	-0.00003267	-0.00001725
BEND	12	11	1		-0.00001774	-0.00003604	-0.00000409	0.00001537
BEND	13	11	1		0.00009388	0.00003918	0.00011048	0.00007912
BEND	14	11	1		0.00004296	0.00008373	0.00004633	0.00004855
TORS	13	11	1	12	0.00000709	-0.00000521	-0.00001732	-0.00001675
TORS	14	11	1	12	0.00006461	0.00000463	-0.00001142	0.00000832
BEND	15	14	11		0.00000389	-0.00000002	0.00000015	0.00000034
TORS	8	7	2	1	-0.01339969	0.00001414	0.00000370	-0.00002056
TORS	11	1	2	7	-0.00433514	0.00009754	0.00024325	-0.00008791
TORS	14	11	1	2	0.00000257	0.00005846	-0.00016364	-0.00006214
TORS	15	14	11	1	0.00000263	-0.00000160	0.00000768	0.00000809

41	42	43	44
3196.3	3345.3	3484.7	3519.8

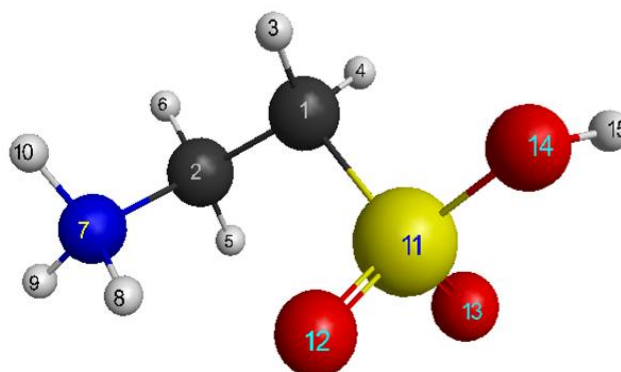
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STR.	15	14			0.00000001	0.00000346	0.00000720	0.00000005
BEND	11	1	2		0.00052147	0.00003907	0.00000257	0.00003184
BEND	3	1	2		0.00023018	0.00000001	0.00000041	0.00000076
BEND	4	1	2		0.00000221	0.00001089	0.00000168	-0.00000010
TORS	3	1	2	11	-0.00000064	0.00000186	0.00000087	0.00000009
TORS	4	1	2	11	-0.00001802	0.00000237	0.00000053	-0.00000028
BEND	7	2	1		-0.00002879	0.00052631	-0.00045632	0.00022357
BEND	5	2	1		-0.00043979	0.00000327	0.00001501	0.00000986
BEND	6	2	1		-0.00100162	0.00004510	0.00000020	0.00000763
TORS	5	2	1	7	-0.00131345	-0.00006795	0.00001855	0.00008125
TORS	6	2	1	7	0.00106625	0.00020202	-0.00000253	-0.00006043
BEND	8	7	2		0.00019695	0.00010034	-0.00075174	-0.00019590
BEND	9	7	2		0.00004478	-0.00021651	0.00225824	0.00052592
BEND	10	7	2		0.00040112	-0.00015569	-0.00007252	0.00058584
TORS	9	7	2	8	-0.00007309	0.00023160	0.00001837	-0.00083908
TORS	10	7	2	8	-0.00001328	-0.00009107	0.00164103	-0.00197537
BEND	12	11	1		-0.00000007	0.00000847	0.00000004	-0.00000054
BEND	13	11	1		-0.00000441	-0.00000052	0.00000189	-0.00000006
BEND	14	11	1		-0.00000667	0.00000238	-0.00000053	-0.00000163
TORS	13	11	1	12	-0.00000031	-0.00000421	0.00000003	-0.00000085
TORS	14	11	1	12	-0.00000179	0.00002120	-0.00000265	0.00000027

BEND	15	14	11		-0.00000001	0.00000043	-0.00000002	-0.00000001
TORS	8	7	2	1	0.00024035	0.00062416	-0.00041059	0.00349515
TORS	11	1	2	7	-0.00039814	0.00014228	-0.00010798	-0.00085903
TORS	14	11	1	2	-0.00005123	0.00000218	0.00001335	-0.00000041
TORS	15	14	11	1	-0.00000009	0.00000010	-0.00000001	0.00000000

45
3713.8

STR.	2	1			-0.00000016
STR.	3	1			0.00000009
STR.	4	1			0.00000118
STR.	5	2			0.00000000
STR.	6	2			0.00000006
STR.	7	2			-0.00000003
STR.	8	7			0.00000611
STR.	9	7			0.00000330
STR.	10	7			0.00000082
STR.	11	1			0.00000007
STR.	12	11			0.00000230
STR.	13	11			0.00002435
STR.	14	11			0.00011559
STR.	15	14			1.00017034
BEND	11	1	2		0.00000021
BEND	3	1	2		0.00000160
BEND	4	1	2		0.00000002
TORS	3	1	2	11	0.00000435
TORS	4	1	2	11	0.00000020
BEND	7	2	1		0.00000003
BEND	5	2	1		0.00000001
BEND	6	2	1		0.00000026
TORS	5	2	1	7	0.00000015
TORS	6	2	1	7	0.00000024
BEND	8	7	2		0.00000057
BEND	9	7	2		0.00000006
BEND	10	7	2		0.00000007
TORS	9	7	2	8	0.00000002
TORS	10	7	2	8	0.00000002
BEND	12	11	1		0.00000035
BEND	13	11	1		0.00000296
BEND	14	11	1		-0.00000418
TORS	13	11	1	12	0.00001523
TORS	14	11	1	12	-0.00016877
BEND	15	14	11		-0.00024842
TORS	8	7	2	1	0.00000004
TORS	11	1	2	7	-0.00000010
TORS	14	11	1	2	0.00003550
TORS	15	14	11	1	0.00003555

S3. DFT calculations of 2-Sea⁺ (g,t)



NO.	TYPE	-- ATOMS --						COORDINATE (BOHR, RAD)	COORDINATE (ANG, DEG)
		I	J	K	L	M	N		
1	STRETCH	2	1					2.8818637	1.5250167
2	STRETCH	3	1					2.0592351	1.0897004
3	STRETCH	4	1					2.0579130	1.0890008
4	STRETCH	5	2					2.0541933	1.0870324
5	STRETCH	6	2					2.0525465	1.0861609
6	STRETCH	7	2					2.8522340	1.5093373
7	STRETCH	8	7					1.9443075	1.0288833
8	STRETCH	9	7					1.9317741	1.0222509
9	STRETCH	10	7					1.9300437	1.0213352
10	STRETCH	11	1					3.3954257	1.7967820
11	STRETCH	12	11					2.7265395	1.4428227
12	STRETCH	13	11					2.7102728	1.4342147
13	STRETCH	14	11					2.9886025	1.5815004
14	STRETCH	15	14					1.8372445	0.9722280
15	BEND	11	1	2				1.9549380	112.0096972
16	BEND	3	1	2				1.9578622	112.1772387
17	BEND	4	1	2				1.9110174	109.4932310
18	TORSION	4	1	2	11			2.0794067	119.1412292
19	TORSION	3	1	2	11			-2.0893523	-119.7110709
20	BEND	7	2	1				1.9479058	111.6067818
21	BEND	5	2	1				1.9561847	112.0811253
22	BEND	6	2	1				1.9042156	109.1035168
23	TORSION	5	2	1	7			-2.1043659	-120.5712864
24	TORSION	6	2	1	7			2.0710351	118.6615704
25	BEND	8	7	2				1.9261298	110.3591092
26	BEND	9	7	2				1.9499405	111.7233583
27	BEND	10	7	2				1.9421509	111.2770482
28	TORSION	9	7	2	8			-2.1109296	-120.9473568
29	TORSION	10	7	2	8			2.0749562	118.8862324
30	BEND	12	11	1				1.8614320	106.6521956
31	BEND	13	11	1				1.9334080	110.7761159
32	BEND	14	11	1				1.7989273	103.0709422
33	TORSION	13	11	1	12			2.2942790	131.4525025
34	TORSION	14	11	1	12			-1.9355433	-110.8984619
35	BEND	15	14	11				1.9549080	112.0079749
36	TORSION	8	7	2	1			-0.8126436	-46.5610511
37	TORSION	11	1	2	7			1.1789811	67.5506437
38	TORSION	14	11	1	2			-2.9260039	-167.6476753
39	TORSION	15	14	11	1			-1.6679221	-95.5648957

TOTAL ENERGY DISTRIBUTION MATRIX M (VIBR. CONTRIBUTIONS SUM TO 100 %)

				1	2	3	4
				0.35071E-04	0.17633E-04	0.15487E-04	0.18899E-04
				I	I	I	
STR.	2	1		0.00000000	0.00000000	0.00000000	0.00000000
STR.	3	1		0.00000000	0.00000000	0.00000000	0.00000000
STR.	4	1		0.00000000	0.00000000	0.00000000	0.00000000
STR.	5	2		0.00000000	0.00000000	0.00000000	0.00000000
STR.	6	2		0.00000000	0.00000000	0.00000000	0.00000000
STR.	7	2		0.00000000	0.00000000	0.00000000	0.00000000
STR.	8	7		0.00000000	0.00000000	0.00000000	0.00000000
STR.	9	7		0.00000000	0.00000000	0.00000000	0.00000000
STR.	10	7		0.00000000	0.00000000	0.00000000	0.00000000
STR.	11	1		0.00000000	0.00000000	0.00000000	0.00000000
STR.	12	11		0.00000000	0.00000000	0.00000000	0.00000000
STR.	13	11		0.00000000	0.00000000	0.00000000	0.00000000
STR.	14	11		0.00000000	0.00000000	0.00000000	0.00000000
STR.	15	14		0.00000000	0.00000000	0.00000000	0.00000000
BEND	11	1	2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	3	1	2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	4	1	2	0.00000000	0.00000000	0.00000000	0.00000000
TORS	4	1	2 11	0.00000000	0.00000000	0.00000000	0.00000000
TORS	3	1	2 11	0.00000000	0.00000000	0.00000000	0.00000000
BEND	7	2	1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	5	2	1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	6	2	1	0.00000000	0.00000000	0.00000000	0.00000000
TORS	5	2	1 7	0.00000000	0.00000000	0.00000000	0.00000000
TORS	6	2	1 7	0.00000000	0.00000000	0.00000000	0.00000000
BEND	8	7	2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	9	7	2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	10	7	2	0.00000000	0.00000000	0.00000000	0.00000000
TORS	9	7	2 8	0.00000000	0.00000000	0.00000000	0.00000000
TORS	10	7	2 8	0.00000000	0.00000000	0.00000000	0.00000000
BEND	12	11	1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	13	11	1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	14	11	1	0.00000000	0.00000000	0.00000000	0.00000000
TORS	13	11	1 12	0.00000000	0.00000000	0.00000000	0.00000000
TORS	14	11	1 12	0.00000000	0.00000000	0.00000000	0.00000000
BEND	15	14	11	0.00000000	0.00000000	0.00000000	0.00000000
TORS	8	7	2 1	0.00000000	0.00000000	0.00000000	0.00000000
TORS	11	1	2 7	0.00000000	0.00000000	0.00000000	0.00000000
TORS	14	11	1 2	0.00000000	0.00000000	0.00000000	0.00000000
TORS	15	14	11 1	0.00000000	0.00000000	0.00000000	0.00000000
				5	6	7	8
				0.20943E-04	0.36443E-04	127.14	176.84
STR.	2	1		0.00000000	0.00000000	0.00113236	-0.00996824
STR.	3	1		0.00000000	0.00000000	-0.00011353	-0.00000009
STR.	4	1		0.00000000	0.00000000	0.00004360	-0.00001212
STR.	5	2		0.00000000	0.00000000	-0.00000276	-0.00000056
STR.	6	2		0.00000000	0.00000000	0.00000322	0.00000011
STR.	7	2		0.00000000	0.00000000	0.00272069	-0.00084246
STR.	8	7		0.00000000	0.00000000	-0.00000415	0.00013139
STR.	9	7		0.00000000	0.00000000	-0.00008396	-0.00001758
STR.	10	7		0.00000000	0.00000000	0.00000013	0.00001773

STR.	11	1			0.00000000	0.00000000	0.00270128	-0.00480900
STR.	12	11			0.00000000	0.00000000	-0.00015787	-0.00035307
STR.	13	11			0.00000000	0.00000000	-0.00024075	0.00047466
STR.	14	11			0.00000000	0.00000000	-0.00031401	0.00112399
STR.	15	14			0.00000000	0.00000000	-0.00000104	-0.00002033
BEND	11	1	2		0.00000000	0.00000000	0.03104278	0.26840258
BEND	3	1	2		0.00000000	0.00000000	-0.00112778	0.00000339
BEND	4	1	2		0.00000000	0.00000000	-0.00191317	-0.00066041
TORS	4	1	2	11	0.00000000	0.00000000	-0.00317886	-0.00004423
TORS	3	1	2	11	0.00000000	0.00000000	-0.00087882	-0.00217122
BEND	7	2	1		0.00000000	0.00000000	-0.00010294	0.08154962
BEND	5	2	1		0.00000000	0.00000000	-0.00005564	0.00002266
BEND	6	2	1		0.00000000	0.00000000	-0.00000004	0.00075684
TORS	5	2	1	7	0.00000000	0.00000000	0.00000790	-0.00119627
TORS	6	2	1	7	0.00000000	0.00000000	-0.00040812	-0.00042923
BEND	8	7	2		0.00000000	0.00000000	0.00065459	0.01458772
BEND	9	7	2		0.00000000	0.00000000	-0.00086756	0.00109066
BEND	10	7	2		0.00000000	0.00000000	0.00008096	-0.00185402
TORS	9	7	2	8	0.00000000	0.00000000	-0.00064358	-0.00277814
TORS	10	7	2	8	0.00000000	0.00000000	-0.00142539	0.00274987
BEND	12	11	1		0.00000000	0.00000000	0.00060153	0.03413091
BEND	13	11	1		0.00000000	0.00000000	0.07177690	0.00721696
BEND	14	11	1		0.00000000	0.00000000	0.03668648	0.10911812
TORS	13	11	1	12	0.00000000	0.00000000	0.02321469	0.01791006
TORS	14	11	1	12	0.00000000	0.00000000	-0.05524663	0.01393747
BEND	15	14	11		0.00000000	0.00000000	-0.00127170	0.00001717
TORS	8	7	2	1	0.00000000	0.00000000	0.00003701	0.00038940
TORS	11	1	2	7	0.00000000	0.00000000	-0.08872650	0.46692592
TORS	14	11	1	2	0.00000000	0.00000000	0.98082188	0.00610126
TORS	15	14	11	1	0.00000000	0.00000000	0.00523881	-0.00150154

9	10	11	12
247.12	290.02	330.70	388.66

STR.	2	1			0.00595661	0.02932539	0.02833501	0.00043223
STR.	3	1			0.00000935	0.00002576	-0.00006916	-0.00004951
STR.	4	1			0.00000441	0.00001465	0.00007297	0.00003689
STR.	5	2			0.00010935	0.00006132	0.00004542	-0.00000508
STR.	6	2			0.00000671	0.00001431	0.00009883	0.00001309
STR.	7	2			0.00078065	0.00217134	0.00093900	-0.00008836
STR.	8	7			-0.00002075	0.00001115	0.00003310	-0.00000318
STR.	9	7			0.00001575	-0.00018701	0.00003137	-0.00001579
STR.	10	7			-0.00001025	0.00000592	-0.00000117	0.00000068
STR.	11	1			0.00099571	0.01370906	0.08919135	0.00324469
STR.	12	11			0.00080035	-0.00016453	0.00003707	0.00225734
STR.	13	11			-0.00006732	0.00044893	-0.00000003	-0.00059910
STR.	14	11			-0.00073268	0.00060817	0.00141607	0.00000251
STR.	15	14			-0.00000099	0.00006990	0.00003107	0.00026851
BEND	11	1	2		0.07384152	0.04698131	0.28413003	0.00417872
BEND	3	1	2		-0.00054083	0.00000150	-0.00063685	0.00007553
BEND	4	1	2		-0.00039151	0.00032254	0.00223730	-0.00056234
TORS	4	1	2	11	-0.00003526	0.00790006	0.00026588	0.01378145
TORS	3	1	2	11	0.00047785	0.00489582	0.01019226	0.02113109
BEND	7	2	1		0.02530183	0.13963618	0.01519725	0.01434885
BEND	5	2	1		0.00100311	-0.00030798	0.00265954	0.00047856
BEND	6	2	1		-0.00104008	0.00221309	0.00144153	-0.00000276
TORS	5	2	1	7	-0.00400522	0.00373393	0.00324520	-0.00029521
TORS	6	2	1	7	0.00247716	0.00041689	0.00182495	0.00002292
BEND	8	7	2		0.00527201	-0.00024950	0.00056577	0.00102196

BEND	9	7	2		-0.00107444	-0.00009934	0.00010185	0.00027969
BEND	10	7	2		-0.00197083	-0.00472318	-0.00079548	-0.00002139
TORS	9	7	2	8	-0.00363784	-0.00019073	0.00003818	0.00014110
TORS	10	7	2	8	0.00227458	-0.00174400	-0.00038318	-0.00014621
BEND	12	11	1		0.06033263	0.29192404	0.08072819	0.05394032
BEND	13	11	1		0.04847772	0.27543539	0.06636715	0.07238956
BEND	14	11	1		0.33096745	0.06441688	0.21829541	0.04504182
TORS	13	11	1	12	-0.03923229	0.01083341	0.00657925	-0.00835501
TORS	14	11	1	12	0.01986609	0.01011955	0.11122794	0.46713190
BEND	15	14	11		-0.00030593	0.00265598	0.00428000	0.02392175
TORS	8	7	2	1	-0.00420920	-0.00169607	-0.00046750	-0.00004946
TORS	11	1	2	7	0.40936238	0.05569678	0.03937107	0.01368477
TORS	14	11	1	2	0.07219929	0.00963731	-0.04957651	-0.02733053
TORS	15	14	11	1	-0.00325705	0.03607579	0.08294990	0.29969803

13	14	15	16
443.28	498.05	544.38	572.57

STR.	2	1			-0.00056527	0.00997376	0.00790933	0.00028636
STR.	3	1			-0.00006797	0.00000757	0.00001058	0.00001199
STR.	4	1			0.00041091	0.00006730	0.00013240	0.00013308
STR.	5	2			0.00009049	-0.00000001	-0.00001370	-0.00002820
STR.	6	2			0.00004192	0.00002374	0.00001195	0.00000307
STR.	7	2			0.00883762	0.00070293	-0.00000024	0.00229571
STR.	8	7			0.00000261	0.00000146	-0.00000143	0.00000402
STR.	9	7			-0.00033837	0.00001096	-0.00001368	-0.00002693
STR.	10	7			-0.00000672	-0.00000019	-0.00000627	-0.00000179
STR.	11	1			0.10968983	0.12804437	-0.00011779	0.03260965
STR.	12	11			0.00028779	0.00234718	0.00028392	0.00136904
STR.	13	11			-0.00000530	0.00232744	0.00341615	0.00311543
STR.	14	11			0.00289785	0.02388210	0.02904033	0.02671757
STR.	15	14			-0.00000533	0.00005929	-0.00029139	-0.00004366
BEND	11	1	2		0.00209838	-0.00028326	0.05206479	0.09801125
BEND	3	1	2		0.01521461	-0.00070465	0.00807909	0.00805083
BEND	4	1	2		0.00126982	-0.00039437	0.00003428	-0.00085295
TORS	4	1	2	11	0.02001340	-0.00223905	0.01018921	-0.00245604
TORS	3	1	2	11	0.02992061	0.00397779	0.01083499	-0.00154621
BEND	7	2	1		0.45934291	0.00862832	0.03680210	0.06991718
BEND	5	2	1		0.00061676	0.00059452	0.00665553	0.01090075
BEND	6	2	1		0.00754587	0.00117357	0.00103043	0.00575952
TORS	5	2	1	7	0.00134795	0.00031200	0.00066825	0.00244289
TORS	6	2	1	7	-0.00346892	0.00040581	0.00094867	0.00271403
BEND	8	7	2		0.02052627	0.00009135	0.00653749	0.00692573
BEND	9	7	2		0.00887847	-0.00000194	0.00286321	0.00272776
BEND	10	7	2		-0.00338186	-0.00003133	-0.00016976	-0.00041578
TORS	9	7	2	8	0.00140454	0.00002139	0.00021831	0.00018909
TORS	10	7	2	8	0.00035546	0.00001737	0.00022540	0.00040883
BEND	12	11	1		-0.01786389	0.11232925	0.05224870	0.17849671
BEND	13	11	1		0.10742158	0.08253308	0.04782729	0.08906323
BEND	14	11	1		0.06648694	0.01370942	0.00038124	-0.03020290
TORS	13	11	1	12	0.06007281	0.60312604	0.18632898	0.03264683
TORS	14	11	1	12	-0.01467160	0.00662118	0.15533977	0.25928976
BEND	15	14	11		0.00013272	0.00066262	-0.00707597	0.00247970
TORS	8	7	2	1	-0.00410044	-0.00032568	0.00145522	0.00058665
TORS	11	1	2	7	0.11806966	-0.00000336	0.00605127	0.00020442
TORS	14	11	1	2	0.00094600	-0.00003711	0.01692020	0.00606796
TORS	15	14	11	1	0.00055187	0.00236917	0.36318115	0.19214542

17	18	19	20
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			702.14	820.71	849.64	853.84
STR.	2	1	0.01542938	0.05107896	0.00001209	0.14064581
STR.	3	1	-0.00002106	0.00011003	0.00002164	0.00005605
STR.	4	1	0.00007082	-0.00020472	-0.00014398	-0.00028427
STR.	5	2	-0.00002425	-0.00000955	-0.00001179	-0.00005790
STR.	6	2	0.00009736	-0.00007700	-0.00001331	-0.00003017
STR.	7	2	0.00457845	0.01047612	0.01186490	0.42957781
STR.	8	7	0.00000218	-0.00001894	-0.00003578	-0.00004047
STR.	9	7	0.00001415	0.00048407	0.00006984	0.00052103
STR.	10	7	0.00000018	-0.00005671	0.00002191	-0.00009469
STR.	11	1	0.47225878	0.00606947	0.07274477	0.00866630
STR.	12	11	0.02263076	0.00250531	0.00126530	0.00082736
STR.	13	11	0.02108140	0.00285066	0.00402639	0.00117609
STR.	14	11	0.04221535	0.27470462	0.55227317	0.01810866
STR.	15	14	0.00003259	0.00006924	0.00013209	-0.00000345
BEND	11	1 2	0.05133264	0.00263045	-0.00189564	0.02822649
BEND	3	1 2	0.00431776	0.03006849	0.03649950	0.01246047
BEND	4	1 2	-0.00054127	-0.00195608	0.00114668	0.03493199
TORS	4	1 2 11	-0.00471402	0.04057743	0.04883962	0.05296057
TORS	3	1 2 11	0.00374820	0.04105138	0.01441402	0.10641705
BEND	7	2 1	0.00383038	-0.00731129	0.00060749	-0.00478483
BEND	5	2 1	0.01613264	0.02237041	0.01557109	0.00952217
BEND	6	2 1	0.03681161	0.00473655	-0.00044407	0.00092602
TORS	5	2 1 7	0.01453409	0.03214808	0.01336153	0.00493365
TORS	6	2 1 7	0.01235175	0.05678593	0.02660325	0.00157295
BEND	8	7 2	0.00291742	0.17201635	0.04209682	-0.00357404
BEND	9	7 2	0.00035170	0.03917126	0.00666519	0.01807720
BEND	10	7 2	-0.00030013	0.00145563	0.00022534	-0.00200504
TORS	9	7 2 8	0.00038449	0.03374208	0.01345061	0.00740651
TORS	10	7 2 8	-0.00013221	-0.01835303	-0.00668974	-0.00266555
BEND	12	11 1	0.07286871	0.00500225	0.00502683	0.03963505
BEND	13	11 1	0.06695539	-0.00022070	0.02808144	0.00331169
BEND	14	11 1	0.12047467	-0.00014436	-0.00097750	0.00019078
TORS	13	11 1 12	0.02694698	0.01561753	0.01871654	0.00849975
TORS	14	11 1 12	-0.00439060	-0.00136051	0.00419723	0.00088461
BEND	15	14 11	-0.00039152	0.00435645	0.00366986	0.00235284
TORS	8	7 2 1	-0.00206887	0.17315433	0.08322425	0.08776115
TORS	11	1 2 7	-0.00002693	0.00539729	0.00523808	-0.00864719
TORS	14	11 1 2	-0.00003039	0.00101068	0.00014927	0.00094836
TORS	15	14 11 1	0.00027144	0.00007183	-0.00000495	0.00158918

			21 916.50	22 983.95	23 1045.3	24 1079.7
STR.	2	1	0.10176710	0.01616041	0.42223750	0.11052903
STR.	3	1	0.00000171	-0.00011407	0.00024449	0.00011541
STR.	4	1	0.00000250	-0.00054677	0.00000059	0.00009887
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STR.	6	2	-0.00005459	0.00000561	0.00015811	0.00065902
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STR.	9	7	-0.00023990	0.00001641	-0.00018898	0.00013718
STR.	10	7	0.00029100	0.00010429	0.00001874	0.00000003
STR.	11	1	0.02940435	0.00136874	0.01224344	0.00065661
STR.	12	11	0.00054270	0.00582599	0.01674402	0.04744361
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STR.	14	11	0.00472291	0.00016010	-0.00004226	0.00036910
STR.	15	14	-0.00000047	0.00000361	0.00000737	0.00000092

BEND	11	1	2	0.02258305	0.00010845	-0.00288643	0.04157225
BEND	3	1	2	0.00506211	-0.00719202	0.02942270	0.00313177
BEND	4	1	2	0.00109652	-0.00068121	0.01611917	-0.00000678
TORS	4	1	2 11	0.00487565	0.15024883	0.03302395	-0.00271167
TORS	3	1	2 11	-0.00113469	0.25441427	-0.00052673	0.01814854
BEND	7	2	1	-0.00325043	0.09140640	0.02224690	0.01280449
BEND	5	2	1	0.00540729	-0.00126731	-0.00236810	0.12348639
BEND	6	2	1	0.01560994	0.01651268	0.11113332	0.19035022
TORS	5	2	1 7	0.03306574	0.06383272	0.00024887	0.05019670
TORS	6	2	1 7	0.03992886	0.04157486	0.03174338	0.04302417
BEND	8	7	2	0.04821961	0.04731554	0.16166536	0.12749503
BEND	9	7	2	-0.00020933	0.01207919	0.00071452	0.03576551
BEND	10	7	2	0.01133176	0.00659674	0.01145556	-0.00147050
TORS	9	7	2 8	0.01529553	0.00822267	0.00437851	-0.00276054
TORS	10	7	2 8	0.04119351	-0.00021639	0.01501789	0.01482297
BEND	12	11	1	0.00082146	0.02195617	-0.00106174	0.00434273
BEND	13	11	1	0.00497370	0.01696089	0.00090957	0.00305744
BEND	14	11	1	0.00363498	0.00004336	0.00087122	0.01079328
TORS	13	11	1 12	0.00181911	-0.00006101	0.00091888	0.00405663
TORS	14	11	1 12	0.00279362	0.00314699	-0.00099577	-0.00050760
BEND	15	14	11	-0.00002683	0.00210322	0.00048763	0.00025312
TORS	8	7	2 1	0.53381233	0.00689844	0.00527954	0.03201223
TORS	11	1	2 7	0.00634568	-0.00492140	0.00036631	0.00274994
TORS	14	11	1 2	0.00456923	-0.01668617	-0.00272140	0.00039156
TORS	15	14	11 1	0.00015062	0.00055703	-0.00000726	0.00002536

25	26	27	28
1164.2	1209.7	1222.4	1320.2

STR.	2	1	-0.00012771	-0.00002542	0.00479141	0.02049352
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STR.	4	1	0.00000233	-0.00002080	0.00001764	-0.00013220
STR.	5	2	0.00000011	0.00000277	0.00000759	0.00030102
STR.	6	2	0.00004725	0.00000010	0.00004940	0.00012485
STR.	7	2	0.00404857	-0.00000405	-0.00034725	0.00909032
STR.	8	7	0.00021499	-0.00000782	-0.00001491	0.00032036
STR.	9	7	0.00004672	0.00014735	0.00065504	0.00092159
STR.	10	7	-0.00000085	-0.00004506	-0.00011996	-0.00006244
STR.	11	1	0.01833935	0.00051941	-0.00015017	0.00026646
STR.	12	11	0.52049833	0.00834816	0.01180576	0.07444501
STR.	13	11	0.26608436	0.07384586	0.07152575	0.13420390
STR.	14	11	0.00279859	0.01721270	0.00213502	-0.00030502
STR.	15	14	0.00000988	-0.00037368	-0.00007944	-0.00000444
BEND	11	1 2	0.01347746	0.00508634	-0.00065576	-0.00033425
BEND	3	1 2	0.00181640	0.07633816	0.20158199	0.16109506
BEND	4	1 2	0.00468774	0.03071797	0.07159442	0.06978615
TORS	4	1 2 11	0.00401150	0.01576371	0.03942233	0.03768878
TORS	3	1 2 11	0.00552178	0.00601084	0.03042383	0.01581418
BEND	7	2 1	0.00169942	0.00024204	-0.00632946	0.03502502
BEND	5	2 1	0.00484965	0.02112259	0.05714055	0.04917690
BEND	6	2 1	0.00894864	0.00040572	0.00024085	0.08912684
TORS	5	2 1 7	0.00199982	0.01046871	0.04846495	0.00735551
TORS	6	2 1 7	0.00104529	0.00206725	0.01329721	0.04455710
BEND	8	7 2	0.01449499	0.00350000	0.00124112	0.01548426
BEND	9	7 2	0.01144530	0.04981039	0.22249188	0.20358065
BEND	10	7 2	0.00001696	0.00914180	0.02828163	0.00903996
TORS	9	7 2 8	0.00032454	0.00692937	0.02114018	0.00446951
TORS	10	7 2 8	0.00317993	0.00187308	0.01298803	0.01693217
BEND	12	11 1	0.00075611	-0.00043432	-0.00065280	-0.00010661

BEND	13	11	1	0.00301870	0.00130892	-0.00012333	-0.00128882
BEND	14	11	1	0.01443516	-0.00530313	0.00011724	0.00063637
TORS	13	11	1 12	0.00921589	0.01525983	0.00307971	-0.00029553
TORS	14	11	1 12	0.00191300	-0.00127141	-0.00116314	0.00439958
BEND	15	14	11	0.07989670	0.64099924	0.16827867	0.00744976
TORS	8	7	2 1	0.00157556	-0.00267306	-0.00737100	-0.00881328
TORS	11	1	2 7	-0.00104080	-0.00012020	0.00137188	-0.00233700
TORS	14	11	1 2	0.00000321	-0.00118600	-0.00061583	0.00132008
TORS	15	14	11 1	0.00075096	0.01433373	0.00553700	0.00010313

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1330.7	1357.4	1377.8	1455.8

STR.	2	1	0.00912919	0.00081313	0.00288257	0.02075784
STR.	3	1	-0.00000854	0.00021954	-0.00007607	0.00008199
STR.	4	1	0.00001044	-0.00000082	-0.00016121	0.00002238
STR.	5	2	0.00021274	0.00030965	0.00005757	-0.00018292
STR.	6	2	0.00018855	0.00004304	-0.00000576	-0.00016716
STR.	7	2	-0.00524233	0.00131351	-0.00392682	-0.00073389
STR.	8	7	0.00021200	0.00006671	0.00025225	0.00001497
STR.	9	7	0.00013745	0.00038210	0.00008911	0.00036202
STR.	10	7	-0.00030291	-0.00016431	-0.00007827	-0.00006123
STR.	11	1	-0.00068078	-0.00079152	0.00375381	-0.00064344
STR.	12	11	0.07347692	0.19086264	0.01404291	0.00021635
STR.	13	11	0.12841974	0.19436940	0.06036835	0.00036675
STR.	14	11	-0.00025443	-0.00036520	0.00138586	-0.00001363
STR.	15	14	-0.00000854	-0.00002058	-0.00000975	0.00000027
BEND	11	1 2	-0.00554172	-0.00559918	-0.01474652	0.00112849
BEND	3	1 2	0.01219470	0.24687222	0.00528395	0.03740557
BEND	4	1 2	0.01009221	-0.00060005	0.11338037	0.00060329
TORS	4	1 2 11	0.05696759	0.01213132	0.33682051	-0.00018101
TORS	3	1 2 11	0.01006462	0.11769132	0.20747768	0.00013310
BEND	7	2 1	0.00486891	0.00231134	-0.00297438	0.01898905
BEND	5	2 1	-0.00172138	0.01073612	0.00018677	0.62588862
BEND	6	2 1	0.16182218	0.01319938	0.15211880	0.14232334
TORS	5	2 1 7	0.05366064	0.01798322	-0.00071873	0.00855487
TORS	6	2 1 7	0.22451313	0.00777714	0.05168024	0.05401267
BEND	8	7 2	0.14038136	0.02837461	0.02264738	0.00295570
BEND	9	7 2	0.08331616	0.10300485	0.02511472	0.08618759
BEND	10	7 2	0.00386079	0.01146039	0.00104559	-0.00016843
TORS	9	7 2 8	0.00567875	0.01418264	0.00542068	-0.00070789
TORS	10	7 2 8	0.00012308	-0.00028931	-0.00007734	0.00294436
BEND	12	11 1	-0.00055687	-0.00058262	0.00409944	0.00016347
BEND	13	11 1	-0.00041296	0.00505425	-0.00057526	0.00002379
BEND	14	11 1	-0.00005814	0.00036258	-0.00005035	0.00049974
TORS	13	11 1 12	0.00067469	-0.00030659	0.00103271	0.00019509
TORS	14	11 1 12	0.00777330	0.00937129	0.00174777	0.00001244
BEND	15	14 11	0.02404471	0.02916779	0.01181542	0.00000004
TORS	8	7 2 1	-0.00125910	-0.00727214	0.00031620	-0.00073897
TORS	11	1 2 7	0.00462562	-0.00266231	0.00006477	-0.00004485
TORS	14	11 1 2	0.00006406	0.00099660	0.00045997	-0.00019535
TORS	15	14 11 1	-0.00046582	-0.00040215	-0.00014496	-0.00000502

33	34	35	36
1525.1	1546.2	1629.8	1754.2

STR.	2	1	0.00335056	0.00640768	-0.00009394	0.00028042
STR.	3	1	0.00000772	-0.00063441	0.00001138	0.00002042
STR.	4	1	-0.00001462	0.00010677	-0.00000001	0.00000004

STR.	5	2			-0.00018707	0.00000459	0.00006237	0.00006312
STR.	6	2			-0.00024125	0.00008023	-0.00000392	0.00006091
STR.	7	2			-0.00756725	-0.00028164	-0.00583922	-0.00372241
STR.	8	7			0.00009515	-0.00000128	-0.00027184	-0.00005229
STR.	9	7			0.00007506	0.00000770	-0.00019410	-0.00099960
STR.	10	7			0.00006616	0.00000421	0.00019191	0.00002211
STR.	11	1			0.00012926	0.00055071	0.00000024	-0.00000633
STR.	12	11			0.00012160	-0.00002005	0.00153030	0.00000921
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STR.	15	14			-0.00000001	0.00000018	-0.00000006	-0.00000040
BEND	11	1	2		0.00063817	0.00401968	0.00012544	0.00011995
BEND	3	1	2		0.02164305	0.09147526	0.00013677	0.00056639
BEND	4	1	2		0.00116705	0.64967274	0.00003969	0.00001372
TORS	4	1	2	11	-0.00033413	0.13137635	0.00009771	0.00017246
TORS	3	1	2	11	-0.00021752	0.09440636	0.00001553	0.00020549
BEND	7	2	1		-0.01392272	-0.00049307	0.00018369	-0.00574782
BEND	5	2	1		0.00436581	0.00890889	0.00693163	0.00097905
BEND	6	2	1		0.03168742	0.00451834	-0.00004712	0.00085338
TORS	5	2	1	7	0.60575825	0.01090624	0.01223022	0.00480613
TORS	6	2	1	7	0.33684269	0.00240825	0.00234733	0.00135243
BEND	8	7	2		0.00106318	0.00030375	0.10736129	0.00220315
BEND	9	7	2		0.01556377	0.00047598	0.02034242	0.04510901
BEND	10	7	2		0.00053952	0.00051579	0.29612244	0.41377064
TORS	9	7	2	8	-0.00007275	0.00002868	0.52548364	0.01663013
TORS	10	7	2	8	0.00002017	0.00081847	0.03683722	0.54379117
BEND	12	11	1		0.00011985	0.00082131	0.00062223	0.00004549
BEND	13	11	1		-0.00000267	0.00001599	0.00042072	-0.00004750
BEND	14	11	1		0.00008791	-0.00055831	-0.00000819	-0.00001306
TORS	13	11	1	12	-0.00004430	0.00106510	0.00037050	0.00001789
TORS	14	11	1	12	-0.00000630	-0.00098665	0.00104901	-0.00004754
BEND	15	14	11		0.00001034	0.00020677	0.00008332	-0.00000269
TORS	8	7	2	1	-0.00000207	-0.00013051	0.01519664	-0.01879486
TORS	11	1	2	7	0.00027300	-0.00047852	-0.02300207	-0.00371076
TORS	14	11	1	2	-0.00110853	-0.00603828	0.00097298	0.00205365
TORS	15	14	11	1	-0.00000235	0.00016291	0.00001195	0.00000016

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1898.0	3092.2	3127.2	3166.9

STR.	2	1			0.00000129	0.00047914	0.00012316	0.00004611
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STR.	5	2			0.00003104	0.00251225	0.20613372	0.00407699
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STR.	8	7			0.00002372	0.00000027	0.00138313	0.00001546
STR.	9	7			-0.00027268	0.00000224	0.00000571	0.00000007
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STR.	11	1			-0.00000490	0.00002931	-0.00000521	0.00001420
STR.	12	11			0.00002417	-0.00000002	0.00000022	0.00000892
STR.	13	11			0.00001041	0.00000165	0.00000003	0.00000494
STR.	14	11			-0.00000017	0.00000263	-0.00000011	0.00000000
STR.	15	14			0.00000002	0.00000018	0.00000001	0.00000001
BEND	11	1	2		0.00013022	-0.00031530	0.00002148	0.00004567
BEND	3	1	2		0.00006084	0.00079489	0.00002590	0.00035799
BEND	4	1	2		0.00006487	0.00007836	0.00010514	-0.00061597
TORS	4	1	2	11	-0.00000095	-0.00074748	0.00000394	-0.00047827
TORS	3	1	2	11	-0.00000098	-0.00002076	-0.00006079	-0.00083702

BEND	7	2	1			-0.00103540	-0.00001850	0.00056549	0.00049672
BEND	5	2	1			0.00001319	0.00017133	-0.00018563	0.00010509
BEND	6	2	1			0.00023981	0.00006584	0.00025560	0.00000272
TORS	5	2	1	7		0.00009606	-0.00001625	-0.00074867	0.00000758
TORS	6	2	1	7		0.00001461	-0.00002769	0.00006412	-0.00002953
BEND	8	7	2			0.00563880	0.00000102	0.00028417	0.00000931
BEND	9	7	2			0.00323307	0.00000285	0.00012352	0.00000125
BEND	10	7	2			0.21202676	-0.00000093	-0.00000823	-0.00000674
TORS	9	7	2	8		0.32780289	0.00000042	-0.00001051	-0.00000057
TORS	10	7	2	8		0.33814992	0.00000007	-0.00004212	0.00000007
BEND	12	11	1			-0.00000120	0.00001299	0.00000800	0.00021766
BEND	13	11	1			-0.00000561	0.00005668	-0.00000006	0.00001735
BEND	14	11	1			-0.00000613	0.00005456	0.00000036	-0.00000045
TORS	13	11	1	12		0.00000774	0.00007040	0.00000043	-0.00000340
TORS	14	11	1	12		-0.00000305	-0.00009724	-0.00000150	0.00000480
BEND	15	14	11			-0.00000039	0.00000007	0.00000001	0.00000022
TORS	8	7	2	1		0.11516116	-0.00000138	0.00000009	-0.00000499
TORS	11	1	2	7		0.00021367	-0.00000324	-0.00000876	0.00013651
TORS	14	11	1	2		0.00009108	-0.00027641	-0.00005371	0.00020204
TORS	15	14	11	1		0.00000005	-0.00000086	0.00000111	0.00002519

41	42	43	44
3199.2	3293.5	3453.2	3560.0

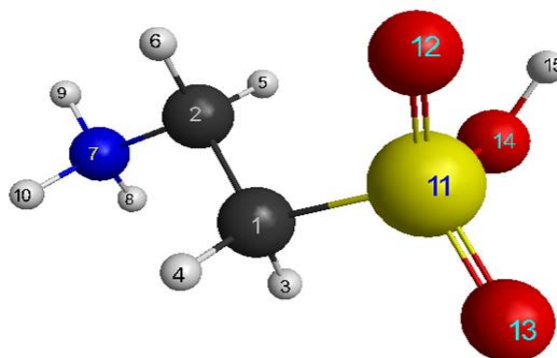
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STR.	6	2				0.19663167	0.00189256	0.00004724	0.00006833
STR.	7	2				0.00001667	-0.00026441	0.00010477	0.00020141
STR.	8	7				0.00055914	0.95942607	0.03361184	0.00421342
STR.	9	7				0.00000166	0.02771973	0.92317509	0.04754681
STR.	10	7				0.00036945	0.01071243	0.04115510	0.94853262
STR.	11	1				0.00000351	0.00000459	-0.00000007	-0.00000001
STR.	12	11				0.00000005	0.00010831	0.00000431	0.00000069
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STR.	14	11				-0.00000019	0.00000281	0.00000043	0.00000007
STR.	15	14				0.00000010	0.00000872	0.00000553	0.00000169
BEND	11	1	2			0.00021303	0.00002972	-0.00000072	0.00001995
BEND	3	1	2			0.00016483	0.00000013	0.00000032	-0.00000003
BEND	4	1	2			-0.00000486	0.00001575	0.00000313	0.00000001
TORS	4	1	2	11		-0.00001519	0.00000351	0.00000050	-0.00000008
TORS	3	1	2	11		0.00000453	0.00000129	0.00000016	0.00000011
BEND	7	2	1			0.00002799	0.00029941	-0.00035975	0.00000169
BEND	5	2	1			-0.00011244	0.00000270	0.00000616	0.00001199
BEND	6	2	1			-0.00033406	0.00005270	0.00000078	0.00000300
TORS	5	2	1	7		0.00048596	-0.00005753	0.00000593	0.00017411
TORS	6	2	1	7		-0.00018870	0.00027433	-0.00000238	-0.00009481
BEND	8	7	2			0.00016543	0.00041730	-0.00046131	-0.00015165
BEND	9	7	2			0.00008412	-0.00038385	0.00395972	0.00002298
BEND	10	7	2			0.00047324	-0.00034052	-0.00024844	0.00047107
TORS	9	7	2	8		-0.00008177	-0.00007025	-0.00004738	-0.00198248
TORS	10	7	2	8		-0.00000078	-0.00010592	-0.00139319	-0.00105926
BEND	12	11	1			0.00000293	-0.00000112	0.00000312	0.00000007
BEND	13	11	1			-0.00000112	0.00000270	0.00000060	-0.00000071
BEND	14	11	1			-0.00000346	0.00000613	-0.00000069	-0.00000045
TORS	13	11	1	12		-0.00000021	0.00000291	0.00000099	0.00000001
TORS	14	11	1	12		0.00000215	0.00000225	0.00000115	-0.00000033
BEND	15	14	11			0.00000000	0.00000127	0.00000005	0.00000001

TORS	8	7	2	1	0.00026310	0.00033208	0.00037248	0.00215069
TORS	11	1	2	7	0.00021124	-0.00012406	0.00002652	-0.00052865
TORS	14	11	1	2	-0.00001758	0.00001044	0.00000685	-0.00000200
TORS	15	14	11	1	0.00000059	0.00000087	0.00000006	0.00000004

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3720.9

STR.	2	1			-0.00000012
STR.	3	1			0.00000032
STR.	4	1			0.00000020
STR.	5	2			0.00000008
STR.	6	2			0.00000001
STR.	7	2			0.00000004
STR.	8	7			0.00001103
STR.	9	7			0.00000239
STR.	10	7			0.00000210
STR.	11	1			-0.00000001
STR.	12	11			0.00002395
STR.	13	11			0.00000252
STR.	14	11			0.00017399
STR.	15	14			1.00016240
BEND	11	1	2		-0.00000151
BEND	3	1	2		0.00000000
BEND	4	1	2		0.00000007
TORS	4	1	2	11	0.00000000
TORS	3	1	2	11	0.00000004
BEND	7	2	1		-0.00000010
BEND	5	2	1		0.00000001
BEND	6	2	1		0.00000160
TORS	5	2	1	7	0.00000020
TORS	6	2	1	7	0.00000005
BEND	8	7	2		0.00000067
BEND	9	7	2		0.00000003
BEND	10	7	2		0.00000004
TORS	9	7	2	8	0.00000001
TORS	10	7	2	8	0.00000001
BEND	12	11	1		0.00000304
BEND	13	11	1		0.00000006
BEND	14	11	1		0.00001504
TORS	13	11	1	12	0.00001696
TORS	14	11	1	12	-0.00008301
BEND	15	14	11		-0.00025242
TORS	8	7	2	1	0.00000004
TORS	11	1	2	7	-0.00000019
TORS	14	11	1	2	-0.00006816
TORS	15	14	11	1	-0.00001138

S4. DFT calculations of 2-Sea⁺ (*t,g*)



NO.	TYPE	-- ATOMS --						COORDINATE (BOHR, RAD)	COORDINATE (ANG, DEG)
		I	J	K	L	M	N		
1	STRETCH	2	1					2.8796260	1.5238326
2	STRETCH	3	1					2.0602487	1.0902367
3	STRETCH	4	1					2.0610271	1.0906487
4	STRETCH	5	2					2.0510285	1.0853576
5	STRETCH	6	2					2.0525708	1.0861738
6	STRETCH	7	2					2.8443085	1.5051433
7	STRETCH	8	7					1.9359489	1.0244601
8	STRETCH	9	7					1.9316548	1.0221878
9	STRETCH	10	7					1.9336168	1.0232260
10	STRETCH	11	1					3.3819368	1.7896440
11	STRETCH	12	11					2.7164277	1.4374718
12	STRETCH	13	11					2.7074716	1.4327324
13	STRETCH	14	11					3.0123759	1.5940808
14	STRETCH	15	14					1.8373643	0.9722914
15	BEND	11	1	2				1.9586505	112.2224049
16	BEND	3	1	2				1.9642591	112.5437538
17	BEND	4	1	2				1.9610180	112.3580577
18	TORSION	3	1	2	11			-2.0796037	-119.1525176
19	TORSION	4	1	2	11			2.0543778	117.7071779
20	BEND	7	2	1				1.9206715	110.0463714
21	BEND	5	2	1				1.9533689	111.9197934
22	BEND	6	2	1				1.9440064	111.3833614
23	TORSION	5	2	1	7			-2.0704231	-118.6265029
24	TORSION	6	2	1	7			2.0697502	118.5879488
25	BEND	8	7	2				1.9559985	112.0704576
26	BEND	9	7	2				1.9338530	110.8016143
27	BEND	10	7	2				1.9547712	112.0001413
28	TORSION	9	7	2	8			-2.1025640	-120.4680407
29	TORSION	10	7	2	8			2.1070010	120.7222669
30	BEND	12	11	1				1.9246013	110.2715300
31	BEND	13	11	1				1.8824163	107.8545076
32	BEND	14	11	1				1.7394849	99.6651455
33	TORSION	13	11	1	12			2.3114855	132.4383617
34	TORSION	14	11	1	12			-1.9927813	-114.1779561
35	BEND	15	14	11				1.9344800	110.8375379
36	TORSION	8	7	2	1			-1.1531901	-66.0729263
37	TORSION	11	1	2	7			3.0976881	177.4844570
38	TORSION	14	11	1	2			-1.1213394	-64.2480163
39	TORSION	15	14	11	1			2.3705738	135.8238711

TOTAL ENERGY DISTRIBUTION MATRIX M (VIBR. CONTRIBUTIONS SUM TO 100 %)

			1	2	3	4
			0.38311E-04	0.36084E-04	0.11838E-04	0.14991E-04
			I	I		
STR.	2	1	0.00000000	0.00000000	0.00000000	0.00000000
STR.	3	1	0.00000000	0.00000000	0.00000000	0.00000000
STR.	4	1	0.00000000	0.00000000	0.00000000	0.00000000
STR.	5	2	0.00000000	0.00000000	0.00000000	0.00000000
STR.	6	2	0.00000000	0.00000000	0.00000000	0.00000000
STR.	7	2	0.00000000	0.00000000	0.00000000	0.00000000
STR.	8	7	0.00000000	0.00000000	0.00000000	0.00000000
STR.	9	7	0.00000000	0.00000000	0.00000000	0.00000000
STR.	10	7	0.00000000	0.00000000	0.00000000	0.00000000
STR.	11	1	0.00000000	0.00000000	0.00000000	0.00000000
STR.	12	11	0.00000000	0.00000000	0.00000000	0.00000000
STR.	13	11	0.00000000	0.00000000	0.00000000	0.00000000
STR.	14	11	0.00000000	0.00000000	0.00000000	0.00000000
STR.	15	14	0.00000000	0.00000000	0.00000000	0.00000000
BEND	11	1 2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	3	1 2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	4	1 2	0.00000000	0.00000000	0.00000000	0.00000000
TORS	3	1 2 11	0.00000000	0.00000000	0.00000000	0.00000000
TORS	4	1 2 11	0.00000000	0.00000000	0.00000000	0.00000000
BEND	7	2 1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	5	2 1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	6	2 1	0.00000000	0.00000000	0.00000000	0.00000000
TORS	5	2 1 7	0.00000000	0.00000000	0.00000000	0.00000000
TORS	6	2 1 7	0.00000000	0.00000000	0.00000000	0.00000000
BEND	8	7 2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	9	7 2	0.00000000	0.00000000	0.00000000	0.00000000
BEND	10	7 2	0.00000000	0.00000000	0.00000000	0.00000000
TORS	9	7 2 8	0.00000000	0.00000000	0.00000000	0.00000000
TORS	10	7 2 8	0.00000000	0.00000000	0.00000000	0.00000000
BEND	12	11 1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	13	11 1	0.00000000	0.00000000	0.00000000	0.00000000
BEND	14	11 1	0.00000000	0.00000000	0.00000000	0.00000000
TORS	13	11 1 12	0.00000000	0.00000000	0.00000000	0.00000000
TORS	14	11 1 12	0.00000000	0.00000000	0.00000000	0.00000000
BEND	15	14 11	0.00000000	0.00000000	0.00000000	0.00000000
TORS	8	7 2 1	0.00000000	0.00000000	0.00000000	0.00000000
TORS	11	1 2 7	0.00000000	0.00000000	0.00000000	0.00000000
TORS	14	11 1 2	0.00000000	0.00000000	0.00000000	0.00000000
TORS	15	14 11 1	0.00000000	0.00000000	0.00000000	0.00000000
			5	6	7	8
			0.22955E-04	0.43770E-04	116.48	145.49
STR.	2	1	0.00000000	0.00000000	-0.00008273	-0.00024370
STR.	3	1	0.00000000	0.00000000	-0.00007440	-0.00008166
STR.	4	1	0.00000000	0.00000000	-0.00004235	0.00001015
STR.	5	2	0.00000000	0.00000000	-0.00004293	0.00000765
STR.	6	2	0.00000000	0.00000000	-0.00003398	-0.00000489
STR.	7	2	0.00000000	0.00000000	0.00022256	0.00395622
STR.	8	7	0.00000000	0.00000000	-0.00001871	0.00001367
STR.	9	7	0.00000000	0.00000000	0.00000020	0.00000238
STR.	10	7	0.00000000	0.00000000	0.00007314	0.00005120
STR.	11	1	0.00000000	0.00000000	0.00021092	0.00980650

STR.	12	11			0.00000000	0.00000000	0.00012735	-0.00023942
STR.	13	11			0.00000000	0.00000000	0.00017287	0.00043474
STR.	14	11			0.00000000	0.00000000	0.00018047	-0.00003879
STR.	15	14			0.00000000	0.00000000	-0.00016062	-0.00030338
BEND	11	1	2		0.00000000	0.00000000	0.00553703	0.21454893
BEND	3	1	2		0.00000000	0.00000000	-0.00270154	-0.00135912
BEND	4	1	2		0.00000000	0.00000000	-0.00303284	-0.00139343
TORS	3	1	2	11	0.00000000	0.00000000	-0.00504934	-0.00154374
TORS	4	1	2	11	0.00000000	0.00000000	-0.00491472	-0.00458691
BEND	7	2	1		0.00000000	0.00000000	0.00479051	0.00034089
BEND	5	2	1		0.00000000	0.00000000	0.00048293	-0.00004935
BEND	6	2	1		0.00000000	0.00000000	-0.00104420	-0.00112617
TORS	5	2	1	7	0.00000000	0.00000000	-0.00082812	0.00042801
TORS	6	2	1	7	0.00000000	0.00000000	-0.00022968	-0.00000940
BEND	8	7	2		0.00000000	0.00000000	-0.00013352	-0.00003460
BEND	9	7	2		0.00000000	0.00000000	0.00035144	0.00004419
BEND	10	7	2		0.00000000	0.00000000	-0.00004718	0.00018593
TORS	9	7	2	8	0.00000000	0.00000000	-0.00008469	-0.00000271
TORS	10	7	2	8	0.00000000	0.00000000	-0.00007151	-0.00027527
BEND	12	11	1		0.00000000	0.00000000	0.05402219	0.06078560
BEND	13	11	1		0.00000000	0.00000000	0.00568097	0.11577947
BEND	14	11	1		0.00000000	0.00000000	0.21711939	0.13758121
TORS	13	11	1	12	0.00000000	0.00000000	0.00531459	0.01356749
TORS	14	11	1	12	0.00000000	0.00000000	-0.02301279	0.02139719
BEND	15	14	11		0.00000000	0.00000000	0.00047254	0.00141305
TORS	8	7	2	1	0.00000000	0.00000000	-0.00263755	0.00206605
TORS	11	1	2	7	0.00000000	0.00000000	0.11085816	0.00690884
TORS	14	11	1	2	0.00000000	0.00000000	0.59664992	0.13231395
TORS	15	14	11	1	0.00000000	0.00000000	0.04197625	0.28964919

9	10	11	12
187.52	280.44	319.05	343.42

STR.	2	1			0.00025255	0.00001801	0.07749961	-0.00008679
STR.	3	1			-0.00000265	0.00000393	-0.00000012	-0.00010174
STR.	4	1			-0.00001252	-0.00001923	-0.00000313	0.00016886
STR.	5	2			0.00000587	0.00039172	-0.00000718	0.00000023
STR.	6	2			-0.00001277	-0.00050113	-0.00003355	-0.00014881
STR.	7	2			0.00869271	0.00394353	0.03294311	-0.00139517
STR.	8	7			0.00001658	-0.00002653	-0.00000138	0.00000031
STR.	9	7			0.00000892	0.00000071	0.00009505	0.00002160
STR.	10	7			0.00020041	0.00038757	0.00001238	0.00000222
STR.	11	1			-0.00219346	0.00157593	0.27967199	0.01430042
STR.	12	11			0.00018150	0.00001230	0.00000075	0.00012342
STR.	13	11			-0.00044793	0.00003495	0.00107725	-0.00001832
STR.	14	11			-0.00066789	0.00002326	-0.00011288	-0.00098546
STR.	15	14			0.00013162	0.00001691	0.00002392	0.00001842
BEND	11	1	2		0.31977343	-0.00107046	0.06038772	0.02970397
BEND	3	1	2		-0.00023082	-0.00085361	-0.00014946	-0.00088080
BEND	4	1	2		-0.00018998	-0.00097918	0.00005616	-0.00161339
TORS	3	1	2	11	-0.00370173	0.00011192	0.00061830	0.01537478
TORS	4	1	2	11	-0.00019190	-0.00018772	0.00018919	0.00725601
BEND	7	2	1		0.06516329	0.00022696	0.34062485	0.10120318
BEND	5	2	1		0.00163803	-0.00090435	-0.00099064	0.00013291
BEND	6	2	1		-0.00010432	0.00467817	-0.00048878	-0.00025097
TORS	5	2	1	7	0.00013908	0.00325908	-0.00226374	-0.00065581
TORS	6	2	1	7	0.00029243	-0.00593839	-0.00142369	-0.00002324
BEND	8	7	2		0.00000247	-0.00751349	0.00086728	-0.00088496
BEND	9	7	2		0.00289815	-0.00022660	0.00204109	0.00239270

BEND	10	7	2		-0.00008700	-0.00920803	0.00281208	0.00065750
TORS	9	7	2	8	0.00028605	-0.00689152	0.00103425	-0.00000937
TORS	10	7	2	8	-0.00028312	-0.00106995	0.00169478	-0.00041623
BEND	12	11	1		0.09953951	0.02793101	-0.00971708	0.39711874
BEND	13	11	1		0.05687972	0.00642262	0.13483558	0.01958053
BEND	14	11	1		-0.04428878	-0.00304902	0.03626071	0.13878401
TORS	13	11	1	12	0.03009772	-0.00136785	-0.00581201	-0.06101212
TORS	14	11	1	12	-0.00299494	0.00452417	0.03037043	0.13581619
BEND	15	14	11		0.00051631	-0.00020647	0.00000047	0.00066211
TORS	8	7	2	1	-0.00131261	0.01174952	0.00078458	0.00287466
TORS	11	1	2	7	0.01925250	0.77803378	-0.00278120	0.10356907
TORS	14	11	1	2	0.03625233	0.19301248	-0.00035159	0.04286840
TORS	15	14	11	1	0.41450124	0.00365500	0.02023493	0.05585296

13	14	15	16
361.72	449.08	492.61	558.06

STR.	2	1			0.01192810	0.01195390	0.00063200	0.02110866
STR.	3	1			0.00000002	-0.00004688	-0.00000618	0.00002499
STR.	4	1			0.00010861	0.00001066	0.00001112	0.00002730
STR.	5	2			-0.00002634	-0.00001822	-0.00000344	0.00000022
STR.	6	2			-0.00010062	-0.00006796	-0.00000108	0.00000104
STR.	7	2			0.00354471	0.00237221	-0.00001052	0.02488520
STR.	8	7			0.00001413	0.00000228	-0.00000008	-0.00000429
STR.	9	7			0.00000378	0.00000023	0.00000015	0.00000161
STR.	10	7			0.00009517	0.00002771	0.00000806	-0.00001091
STR.	11	1			0.00328008	0.01166816	0.00532573	0.00258973
STR.	12	11			-0.00015205	0.00293696	0.00246252	0.00117726
STR.	13	11			-0.00033631	0.00460421	0.00107595	0.01214185
STR.	14	11			-0.00127543	0.00080610	0.04117530	0.00100893
STR.	15	14			0.00053645	0.00017237	0.00001470	0.00001787
BEND	11	1	2		0.07548411	0.02080046	-0.00023839	0.08779786
BEND	3	1	2		0.00425930	0.00203775	0.00016781	-0.00116980
BEND	4	1	2		0.00486741	0.00176227	0.00057972	-0.00152761
TORS	3	1	2	11	0.00067839	0.00840593	0.00537291	-0.00366632
TORS	4	1	2	11	0.00837893	0.00018130	0.01103106	-0.00221668
BEND	7	2	1		0.12525981	0.05562635	0.01063290	0.07626719
BEND	5	2	1		0.00672269	0.00141888	0.00023678	-0.00039620
BEND	6	2	1		0.00021122	0.00040925	0.00001162	-0.00030171
TORS	5	2	1	7	-0.00073029	-0.00018966	-0.00001326	-0.00035025
TORS	6	2	1	7	0.00020209	-0.00019136	-0.00014166	-0.00038003
BEND	8	7	2		0.00000587	-0.00000333	0.00001026	0.00052609
BEND	9	7	2		0.00687069	0.00331605	0.00066454	0.00105434
BEND	10	7	2		0.00056695	0.00030308	0.00011710	0.00156445
TORS	9	7	2	8	0.00096146	0.00044638	0.00015499	0.00059660
TORS	10	7	2	8	0.00031601	0.00015339	0.00013498	0.00092030
BEND	12	11	1		-0.00096122	-0.02365530	0.00247423	0.32560918
BEND	13	11	1		0.24544067	0.11671345	0.00709374	0.16563559
BEND	14	11	1		0.29027069	0.01245588	-0.03392320	0.19802344
TORS	13	11	1	12	0.00289967	0.01569346	0.92160387	0.00936382
TORS	14	11	1	12	0.05095772	0.69925041	-0.02183861	0.06875745
BEND	15	14	11		0.00445952	0.02276069	0.00347632	0.00502042
TORS	8	7	2	1	-0.00101874	0.00184930	0.00009672	0.00069015
TORS	11	1	2	7	-0.00539647	0.00574738	0.00559903	0.00005656
TORS	14	11	1	2	0.03182056	0.01783437	0.00389024	-0.00022297
TORS	15	14	11	1	0.12985269	0.00245191	0.03212207	0.00537868

17	18	19	20
745.88	813.52	869.85	900.00

STR.	2	1	0.00005805	0.00008469	0.07246634	0.13758196
STR.	3	1	-0.00004897	-0.00003076	-0.00007963	-0.00005969
STR.	4	1	-0.00005361	0.00003034	-0.00013876	-0.000062583
STR.	5	2	-0.00000636	0.00000363	-0.00018632	-0.00001545
STR.	6	2	-0.00000171	0.00000110	0.00004744	-0.00007475
STR.	7	2	0.00847255	0.00398670	0.02072549	0.09160359
STR.	8	7	0.00000302	0.00001374	0.00004421	-0.00005671
STR.	9	7	-0.00000083	0.00000028	0.00009247	0.00011132
STR.	10	7	-0.00002442	-0.00003670	-0.00000050	-0.00004059
STR.	11	1	0.42308162	0.17121088	0.03065965	0.01564934
STR.	12	11	0.02107411	0.00000606	0.00089243	0.00346872
STR.	13	11	0.01167473	0.00063798	0.00000543	0.00204476
STR.	14	11	0.31628661	0.57862329	0.03375851	0.00571948
STR.	15	14	0.00013029	0.00012392	-0.00000240	-0.00000971
BEND	11	1 2	0.06897690	0.03937289	0.00346023	0.01498130
BEND	3	1 2	0.00033837	-0.00080796	0.12027047	0.02162145
BEND	4	1 2	-0.00282106	0.00334598	0.01762069	0.07843015
TORS	3	1 2 11	-0.00965520	0.03304598	0.06773741	0.13834869
TORS	4	1 2 11	0.00340994	0.00735639	0.10119121	0.07250135
BEND	7	2 1	0.07392422	0.01169159	0.00360429	-0.00631626
BEND	5	2 1	-0.00030502	0.00207405	0.04640856	0.05330366
BEND	6	2 1	-0.00015513	0.00304014	0.07673115	0.02405852
TORS	5	2 1 7	-0.00049627	0.00133250	0.06873179	0.00545870
TORS	6	2 1 7	-0.00079973	0.00097260	0.04992360	0.02242199
BEND	8	7 2	0.00100482	0.00044437	0.00069434	0.00014563
BEND	9	7 2	0.01428090	0.01424775	0.06789680	0.10276169
BEND	10	7 2	0.00579264	0.00643636	0.02831488	0.01890177
TORS	9	7 2 8	0.00493016	0.00636707	0.04162943	0.04433297
TORS	10	7 2 8	0.00471684	0.00524237	0.02277919	0.02738302
BEND	12	11 1	0.00572521	0.00704259	0.01651624	0.00030442
BEND	13	11 1	0.04241194	0.04271750	-0.00053981	0.00447187
BEND	14	11 1	0.00320357	-0.00163581	0.00130840	0.00630152
TORS	13	11 1 12	0.00033351	0.02199825	0.00237233	0.02535391
TORS	14	11 1 12	0.00093163	-0.00208719	0.00168865	-0.02064575
BEND	15	14 11	-0.00433197	0.03184242	0.00072493	0.00038927
TORS	8	7 2 1	0.00684153	0.00853304	0.11078326	0.12194573
TORS	11	1 2 7	-0.00057314	0.00233101	-0.01824460	0.01496957
TORS	14	11 1 2	-0.00017887	0.00024233	0.01028677	-0.02765602
TORS	15	14 11 1	0.00184911	0.00019863	-0.00017456	0.00093443

21	22	23	24
979.27	1043.0	1063.4	1117.4

STR.	2	1	0.01118515	0.08534128	0.45373967	0.00061444
STR.	3	1	-0.00011456	-0.00003910	0.00014100	0.00001649
STR.	4	1	0.00001198	-0.00041816	-0.00001916	0.00000867
STR.	5	2	0.00016720	-0.00021264	0.00009731	-0.00000645
STR.	6	2	-0.00006640	0.00015463	0.00002633	0.00000452
STR.	7	2	0.61729012	0.04411991	0.14025809	0.00054873
STR.	8	7	0.00017493	-0.00000457	-0.00016535	-0.00000055
STR.	9	7	-0.00000305	-0.00000944	-0.00003927	0.00000031
STR.	10	7	-0.00037825	0.00012854	0.00002528	-0.00000066
STR.	11	1	-0.00003325	0.00383247	0.00130645	0.00069188
STR.	12	11	0.00138117	0.01095103	0.00026353	0.10709145
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STR.	14	11	0.00001011	0.00340366	0.00142939	0.01658546
STR.	15	14	-0.00000608	0.00000837	0.00000814	-0.00081786
BEND	11	1 2	0.07054054	0.00026019	-0.01044531	0.00038655

BEND	3	1	2	0.00008651	-0.00161392	0.02846392	-0.00015046
BEND	4	1	2	0.00122119	0.01792059	0.00121834	0.00008459
TORS	3	1	2 11	0.01810668	0.14570086	0.04418387	0.00246661
TORS	4	1	2 11	0.00767925	0.20718658	0.02536415	0.00233648
BEND	7	2	1	0.07603778	0.00020417	0.02343727	-0.00003477
BEND	5	2	1	-0.00206621	0.02792462	0.05405677	0.00000522
BEND	6	2	1	-0.00453075	0.05787807	-0.00489816	-0.00014430
TORS	5	2	1 7	-0.00949839	0.14707674	0.00271529	0.00377686
TORS	6	2	1 7	-0.00725817	0.14838884	0.00986818	0.00341897
BEND	8	7	2	-0.00184621	0.03867401	0.00271422	0.00117161
BEND	9	7	2	-0.00697486	0.00538748	0.00062222	0.00002808
BEND	10	7	2	0.02347091	0.00429515	-0.00366303	0.00039373
TORS	9	7	2 8	0.01333307	0.00335447	-0.01164339	-0.00000248
TORS	10	7	2 8	0.00121498	-0.00138911	-0.01701577	-0.00025059
BEND	12	11	1	0.00309856	0.02322254	-0.00210611	0.00364170
BEND	13	11	1	0.00457586	-0.00004768	0.01488079	0.00254409
BEND	14	11	1	0.00016467	0.00691480	0.00769108	0.00830092
TORS	13	11	1 12	0.00027812	0.01166905	-0.00545182	-0.00308468
TORS	14	11	1 12	0.00774679	-0.00073429	0.01864034	0.02391753
BEND	15	14	11	0.00148431	0.01307826	0.00373772	0.82212498
TORS	8	7	2 1	0.18762339	-0.00436730	0.19984010	0.00050584
TORS	11	1	2 7	0.01378139	-0.00075121	-0.00130481	0.00056435
TORS	14	11	1 2	-0.02859558	-0.00143148	0.02143663	0.00067072
TORS	15	14	11 1	-0.00031012	-0.00045810	0.00067521	-0.00000697

25	26	27	28
1170.2	1195.7	1220.4	1321.2

STR.	2	1	0.00099575	0.00002625	0.08426810	-0.00138875
STR.	3	1	-0.00000686	-0.00001629	0.00004002	-0.00005040
STR.	4	1	-0.00000759	-0.00002541	0.00003439	0.00001025
STR.	5	2	-0.00002961	-0.00001390	0.00039051	0.00014444
STR.	6	2	0.00010349	0.00021945	-0.00000006	0.00008257
STR.	7	2	-0.00009491	0.00796909	-0.00339893	0.00142923
STR.	8	7	0.00001104	0.00000861	-0.00009786	-0.00003753
STR.	9	7	-0.00000155	-0.00001155	0.00053979	0.00028466
STR.	10	7	-0.00000938	-0.00028541	-0.00024405	-0.00014249
STR.	11	1	0.01164485	0.00234053	0.00108328	0.01181001
STR.	12	11	0.33845803	0.05400311	0.00604417	0.11380166
STR.	13	11	0.35274992	0.09801439	0.00632995	0.02999424
STR.	14	11	0.00437371	-0.00081271	0.00027651	-0.00017608
STR.	15	14	-0.00000999	-0.00000318	0.00000091	-0.00001016
BEND	11	1 2	-0.00015998	0.00466223	0.01629668	-0.02325055
BEND	3	1 2	0.01542214	0.10951154	0.15071292	0.15658604
BEND	4	1 2	0.06241162	0.08653172	0.00293125	0.15729950
TORS	3	1 2 11	0.00858677	0.03790865	0.05189886	0.15180608
TORS	4	1 2 11	0.00684849	0.04609301	0.00655024	0.18006108
BEND	7	2 1	-0.00043574	-0.00526185	0.00025335	0.03957931
BEND	5	2 1	0.01038451	0.07319995	0.07712581	0.00159751
BEND	6	2 1	-0.00026195	0.01645397	0.05868911	0.00911503
TORS	5	2 1 7	0.04338344	0.09003544	0.00067368	0.00394799
TORS	6	2 1 7	0.02359389	0.03698084	0.06119745	0.00475824
BEND	8	7 2	0.02985383	0.07232760	0.04193849	0.00727838
BEND	9	7 2	0.00015598	0.02055971	0.26221592	0.09709676
BEND	10	7 2	0.01233348	0.06108796	0.01026120	0.00376996
TORS	9	7 2 8	0.00206913	-0.00007300	-0.03101202	-0.00218540
TORS	10	7 2 8	-0.00512611	-0.03070221	-0.03226210	-0.00945732
BEND	12	11 1	0.00117312	0.00002033	0.00357452	-0.00088907
BEND	13	11 1	0.00510840	0.00045115	0.00441510	0.00007258

BEND	14	11	1		0.00867777	0.00678003	-0.00071135	0.00389384
TORS	13	11	1	12	0.00272198	0.01399606	0.00116421	-0.00050908
TORS	14	11	1	12	0.00054508	-0.00887909	-0.00344759	-0.00271948
BEND	15	14	11		0.04003771	0.02395391	0.00008875	0.00924349
TORS	8	7	2	1	0.02110711	0.17531655	0.23659159	0.05249739
TORS	11	1	2	7	-0.00369383	0.01108774	-0.00378695	-0.00227760
TORS	14	11	1	2	0.00586443	-0.00345773	-0.01092575	0.00692920
TORS	15	14	11	1	0.00122182	0.00000249	0.00029990	0.00000447

29	30	31	32
1348.0	1358.9	1451.0	1506.6

STR.	2	1			0.00874021	-0.00052526	0.00744319	0.00589633
STR.	3	1			0.00026643	0.00004442	-0.00000476	0.00002484
STR.	4	1			-0.00001727	-0.00000074	0.00004926	0.00000455
STR.	5	2			0.00020341	0.00000310	0.00001312	0.00002512
STR.	6	2			0.00026396	0.00002938	0.00032594	0.00064075
STR.	7	2			0.00047699	0.00000282	-0.00133164	-0.00223020
STR.	8	7			-0.00001891	-0.00000767	0.00014208	0.00038814
STR.	9	7			0.00011015	0.00006117	-0.00005169	0.00012913
STR.	10	7			-0.00005602	0.00000162	-0.00064396	-0.00004278
STR.	11	1			0.00073655	0.00063653	-0.00015468	-0.00065262
STR.	12	11			0.01129837	0.32362078	0.00024884	0.00069915
STR.	13	11			0.03823597	0.43294388	0.00050540	0.00004243
STR.	14	11			0.00036577	-0.00002393	0.00006425	0.00000565
STR.	15	14			0.00000364	-0.00001415	-0.00000169	0.00000000
BEND	11	1	2		0.00042376	0.00871573	-0.00144379	-0.00264890
BEND	3	1	2		0.14101890	0.09317041	0.00240038	0.00016071
BEND	4	1	2		0.23026117	0.00121598	0.00009273	0.00082195
TORS	3	1	2	11	0.02341451	0.03281564	0.02069430	0.00824625
TORS	4	1	2	11	0.02860005	0.00406941	0.01867354	0.00996356
BEND	7	2	1		0.00034165	0.00530107	0.00523537	0.00728063
BEND	5	2	1		0.16187954	0.02296351	0.31655142	0.07462267
BEND	6	2	1		0.23601785	0.00938390	0.05708371	0.42886015
TORS	5	2	1	7	-0.00371004	0.00180217	0.18483055	0.04692383
TORS	6	2	1	7	-0.00570854	-0.00008786	0.02281070	0.08099135
BEND	8	7	2		0.08984791	0.00661187	0.19971172	0.30877673
BEND	9	7	2		0.01701614	0.01575054	0.00587870	0.03135204
BEND	10	7	2		0.02009047	0.00004702	0.06480688	0.00197449
TORS	9	7	2	8	0.01643027	-0.00067223	0.08171649	-0.00043059
TORS	10	7	2	8	0.00032482	-0.00093904	0.00378468	0.00478170
BEND	12	11	1		0.00027618	0.00481164	0.00009445	0.00016968
BEND	13	11	1		0.00128855	0.00276693	0.00011071	0.00001637
BEND	14	11	1		-0.00093283	-0.00010051	0.00013748	0.00003507
TORS	13	11	1	12	-0.00005800	-0.00099082	0.00003237	0.00005060
TORS	14	11	1	12	0.00432482	0.01758740	-0.00040101	-0.00005205
BEND	15	14	11		0.00076257	0.01841349	0.00006643	0.00006604
TORS	8	7	2	1	-0.00445332	0.00266078	0.02727036	0.00412454
TORS	11	1	2	7	-0.00091572	0.00031805	-0.01335329	-0.01105143
TORS	14	11	1	2	-0.01714848	-0.00224271	-0.00342584	0.00003403
TORS	15	14	11	1	-0.00000146	-0.00014432	0.00003727	0.00000008

33	34	35	36
1532.1	1552.2	1624.8	1770.5

STR.	2	1			0.00594039	0.00252554	0.00123588	0.00007787
STR.	3	1			-0.00038508	-0.00009686	0.00000009	0.00000103
STR.	4	1			-0.00006154	0.00001806	0.00001504	-0.00000047
STR.	5	2			-0.00003103	-0.00009007	0.00000668	0.00010266

STR.	6	2			-0.00017148	-0.00021334	0.00011727	-0.00000050
STR.	7	2			0.00003205	-0.00990009	0.00145106	-0.00026909
STR.	8	7			0.00000312	0.00004661	-0.00014021	-0.00027609
STR.	9	7			0.00000177	-0.00003150	-0.00101737	0.00100418
STR.	10	7			0.00000412	0.00000611	0.00070651	0.00064379
STR.	11	1			-0.00013444	0.00003408	0.00007989	0.00002299
STR.	12	11			0.00005241	0.00000027	-0.00000062	0.00000264
STR.	13	11			0.00009898	0.00002055	0.00001225	0.00000363
STR.	14	11			-0.00000001	-0.00000071	0.00000023	0.00000175
STR.	15	14			-0.00000025	-0.00000014	0.00000002	0.00000025
BEND	11	1	2		-0.00305807	-0.00025895	0.00023589	0.00033643
BEND	3	1	2		0.10196457	0.05946334	0.00189799	0.00002293
BEND	4	1	2		0.25546739	0.08624686	0.00088045	0.00023456
TORS	3	1	2	11	0.16095069	0.04807841	0.00000547	-0.00001456
TORS	4	1	2	11	0.20276032	0.05594154	-0.00000527	0.00000076
BEND	7	2	1		-0.00458557	-0.00735950	-0.00349632	-0.00052433
BEND	5	2	1		0.05161251	0.01827915	0.00010753	0.00173696
BEND	6	2	1		0.00741743	0.00137214	0.01882331	0.00321874
TORS	5	2	1	7	0.09709169	0.31613520	0.00022004	0.00032816
TORS	6	2	1	7	0.12485462	0.41430922	0.01485610	0.00000140
BEND	8	7	2		0.00001226	0.00829240	0.14370014	0.01325944
BEND	9	7	2		0.00005046	0.00024340	0.30910325	0.02228647
BEND	10	7	2		-0.00002477	0.00295808	0.27324476	0.23766858
TORS	9	7	2	8	0.00009681	0.00031049	0.03097094	0.81773019
TORS	10	7	2	8	0.00006442	0.00147956	0.23055475	-0.02683490
BEND	12	11	1		0.00024539	-0.00021150	0.00000466	0.00000133
BEND	13	11	1		0.00068996	0.00001870	0.00004571	-0.00001635
BEND	14	11	1		0.00032941	0.00011480	0.00005042	-0.00000101
TORS	13	11	1	12	-0.00018813	-0.00000434	0.00002545	0.00001135
TORS	14	11	1	12	0.00044257	0.00004745	-0.00003319	-0.00011608
BEND	15	14	11		0.00000286	0.00000043	0.00000012	-0.00000165
TORS	8	7	2	1	0.00004854	0.00237841	-0.02302631	-0.07157800
TORS	11	1	2	7	-0.00011867	-0.00006919	-0.00072948	0.00219500
TORS	14	11	1	2	-0.00164538	-0.00003312	0.00009121	-0.00126005
TORS	15	14	11	1	0.00016967	-0.00005148	0.00000568	0.00000000

37	38	39	40
2101.7	3072.5	3115.8	3130.1

STR.	2	1			0.00004038	0.00045720	0.00017736	0.00004508
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STR.	5	2			0.00007055	0.00933576	0.55613637	0.02192665
STR.	6	2			0.00000672	0.00298912	0.43084948	0.01655796
STR.	7	2			-0.00014459	-0.00001960	0.00001977	0.00000124
STR.	8	7			-0.00048374	0.00000729	0.00034008	0.00003547
STR.	9	7			0.00020330	0.00000139	0.00000528	0.00000010
STR.	10	7			0.00025546	0.00000868	0.00017130	0.00001137
STR.	11	1			-0.00000049	-0.00007698	-0.00000903	0.00000133
STR.	12	11			0.00000005	0.00000023	0.00000085	0.00000707
STR.	13	11			-0.00000014	0.00000346	-0.00000019	0.00000041
STR.	14	11			-0.00000066	0.00000129	0.00000070	0.00000352
STR.	15	14			-0.00000033	0.00000069	0.00000050	0.00000028
BEND	11	1	2		0.00000370	-0.00026690	0.00013430	0.00001415
BEND	3	1	2		-0.00000908	-0.00017827	0.00004300	0.00031426
BEND	4	1	2		0.00001201	0.00002062	0.00004620	-0.00022996
TORS	3	1	2	11	-0.00000494	-0.00075774	0.00000184	-0.00015204
TORS	4	1	2	11	-0.00000700	0.00005610	-0.00001337	-0.00156416
BEND	7	2	1		-0.00020566	0.00020222	-0.00013373	-0.00000139

BEND	5	2	1		0.00014899	0.00012694	-0.00003226	0.00025361
BEND	6	2	1		-0.00000978	-0.00000114	-0.00004597	0.00027819
TORS	5	2	1	7	0.00094074	-0.00000344	-0.00019699	-0.00012563
TORS	6	2	1	7	0.00069125	-0.00007826	-0.00079781	0.00004900
BEND	8	7	2		0.04204121	0.00000026	0.00004398	-0.00000996
BEND	9	7	2		-0.00151536	0.00001368	0.00041835	0.00000222
BEND	10	7	2		0.23043814	-0.00000410	0.00011754	-0.00000485
TORS	9	7	2	8	-0.01132176	0.00000080	-0.00002809	0.00000811
TORS	10	7	2	8	0.82126107	-0.00000278	-0.00003494	0.00000027
BEND	12	11	1		0.00000221	0.00000628	-0.00000018	0.00013352
BEND	13	11	1		-0.00000066	-0.00002483	-0.00000686	-0.00001571
BEND	14	11	1		-0.00001452	0.00017366	-0.00001698	0.00010612
TORS	13	11	1	12	0.00001405	-0.00001959	0.00000004	-0.00007556
TORS	14	11	1	12	-0.00003490	0.00004620	-0.00000482	0.00000867
BEND	15	14	11		0.00000029	-0.00000001	0.00000037	0.00000092
TORS	8	7	2	1	-0.07102664	0.00001796	0.00003498	-0.00005047
TORS	11	1	2	7	-0.01010671	-0.00001146	0.00013488	-0.00010354
TORS	14	11	1	2	-0.00124138	0.00011659	-0.00000888	-0.00015673
TORS	15	14	11	1	-0.00000042	0.00000533	-0.00000008	-0.00001200

41	42	43	44
3178.8	3412.9	3478.9	3561.6

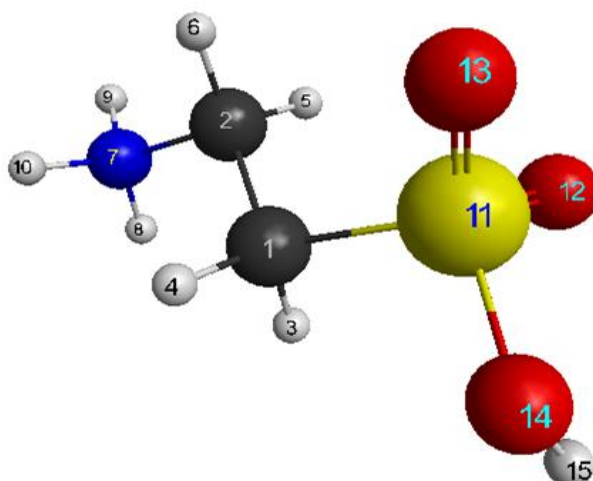
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STR.	3	1			0.02355837	0.00000933	0.00000081	0.00000010
STR.	4	1			0.01479126	0.00000006	0.00000018	0.00000150
STR.	5	2			0.41129493	0.00004416	0.00000530	0.00031257
STR.	6	2			0.54829404	0.00036169	0.00033750	0.00001865
STR.	7	2			0.00000018	-0.00013735	0.00000722	-0.00002329
STR.	8	7			0.00030464	0.58858871	0.39339341	0.01778639
STR.	9	7			0.00001287	0.37814738	0.60433398	0.01599109
STR.	10	7			0.00015150	0.03306120	0.00021712	0.96566268
STR.	11	1			-0.00000090	0.00000042	-0.00000029	0.00000023
STR.	12	11			0.00000078	0.00000013	0.00000001	0.00000003
STR.	13	11			0.00000006	0.00000061	0.00000000	0.00000010
STR.	14	11			0.00000062	0.00000006	0.00000000	0.00000000
STR.	15	14			0.00000036	0.00000432	0.00000000	0.00000221
BEND	11	1	2		-0.00002775	0.00001735	0.00000090	0.00001720
BEND	3	1	2		0.00016562	0.00000398	0.00000057	-0.00000011
BEND	4	1	2		0.00020246	0.00000007	0.00000026	0.00000286
TORS	3	1	2	11	-0.00001476	0.00000024	0.00000053	0.00000010
TORS	4	1	2	11	0.00000434	0.00000010	0.00000008	0.00000006
BEND	7	2	1		-0.00001526	-0.00008929	0.00055866	0.00067170
BEND	5	2	1		-0.00026661	-0.00000004	0.00000000	0.00001498
BEND	6	2	1		-0.00038534	0.00000672	0.00001041	-0.00000014
TORS	5	2	1	7	-0.00038307	-0.00000634	0.00002037	0.00019988
TORS	6	2	1	7	0.00235640	0.00006466	0.00009762	-0.00003369
BEND	8	7	2		0.00045939	-0.00002066	-0.00001029	0.00004040
BEND	9	7	2		0.00007283	0.00000717	0.00162733	0.00000773
BEND	10	7	2		0.00042209	0.00047426	0.00001588	-0.00048437
TORS	9	7	2	8	0.00003729	-0.00096180	0.00009557	-0.00157395
TORS	10	7	2	8	0.00000638	0.00000970	-0.00036061	-0.00033170
BEND	12	11	1		-0.00000680	0.00000000	0.00000002	-0.00000010
BEND	13	11	1		0.00000179	0.00000025	-0.00000014	-0.00000057
BEND	14	11	1		-0.00001362	0.00000059	0.00000001	-0.00000106
TORS	13	11	1	12	-0.00000653	0.00000003	-0.00000001	-0.00000023
TORS	14	11	1	12	0.00000328	-0.00000013	-0.00000004	-0.00000012
BEND	15	14	11		0.00000004	-0.00000001	0.00000000	0.00000000
TORS	8	7	2	1	-0.00004298	0.00067814	-0.00016400	0.00076770

TORS	11	1	2	7	-0.00062498	-0.00027765	-0.00019064	0.00095508
TORS	14	11	1	2	-0.00035164	0.00001433	0.00000324	-0.00000335
TORS	15	14	11	1	0.00000144	0.00000006	0.00000000	-0.00000002

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3714.1

STR.	2	1			0.00000001
STR.	3	1			0.00000091
STR.	4	1			-0.00000004
STR.	5	2			0.00000079
STR.	6	2			0.00000000
STR.	7	2			0.00000029
STR.	8	7			0.00000173
STR.	9	7			0.00000098
STR.	10	7			0.00000299
STR.	11	1			0.00000367
STR.	12	11			0.00000293
STR.	13	11			0.00001415
STR.	14	11			-0.00001009
STR.	15	14			1.00012379
BEND	11	1	2		-0.00000137
BEND	3	1	2		0.00000009
BEND	4	1	2		0.00000067
TORS	3	1	2	11	-0.00000030
TORS	4	1	2	11	0.00000321
BEND	7	2	1		0.00000050
BEND	5	2	1		-0.00000004
BEND	6	2	1		0.00000000
TORS	5	2	1	7	0.00000009
TORS	6	2	1	7	0.00000008
BEND	8	7	2		0.00000003
BEND	9	7	2		0.00000002
BEND	10	7	2		0.00000002
TORS	9	7	2	8	0.00000002
TORS	10	7	2	8	0.00000004
BEND	12	11	1		0.00000229
BEND	13	11	1		0.00000200
BEND	14	11	1		0.00000919
TORS	13	11	1	12	0.00001886
TORS	14	11	1	12	-0.00000190
BEND	15	14	11		-0.00026063
TORS	8	7	2	1	0.00000000
TORS	11	1	2	7	0.00000021
TORS	14	11	1	2	0.00000583
TORS	15	14	11	1	0.00007900

S5. DFT calculations of 2-Sea⁺ (*t,t*)



NO.	TYPE	- - ATOMS - -						COORDINATE (BOHR, RAD)	COORDINATE (ANG, DEG)
		I	J	K	L	M	N		
1	STRETCH	2	1					2.8820181	1.5250984
2	STRETCH	3	1					2.0587484	1.0894428
3	STRETCH	4	1					2.0573699	1.0887133
4	STRETCH	5	2					2.0500412	1.0848352
5	STRETCH	6	2					2.0525948	1.0861865
6	STRETCH	7	2					2.8413897	1.5035988
7	STRETCH	8	7					1.9314714	1.0220907
8	STRETCH	9	7					1.9340159	1.0234372
9	STRETCH	10	7					1.9305941	1.0216265
10	STRETCH	11	1					3.3930053	1.7955012
11	STRETCH	12	11					2.7144718	1.4364367
12	STRETCH	13	11					2.7068998	1.4324298
13	STRETCH	14	11					3.0007899	1.5879497
14	STRETCH	15	14					1.8366223	0.9718987
15	BEND	11	1	2				1.9275153	110.4384928
16	BEND	3	1	2				1.9440325	111.3848567
17	BEND	4	1	2				1.9685639	112.7904029
18	TORSION	3	1	2	11			-2.0392062	-116.8379081
19	TORSION	4	1	2	11			2.0817293	119.2743029
20	BEND	7	2	1				1.9124554	109.5756212
21	BEND	5	2	1				1.9540314	111.9577534
22	BEND	6	2	1				1.9474791	111.5823307
23	TORSION	5	2	1	7			-2.0845164	-119.4339919
24	TORSION	6	2	1	7			2.0635694	118.2338168
25	BEND	8	7	2				1.9481017	111.6180055
26	BEND	9	7	2				1.9334656	110.7794172
27	BEND	10	7	2				1.9502951	111.7436753
28	TORSION	9	7	2	8			-2.0687452	-118.5303662
29	TORSION	10	7	2	8			2.1451653	122.9089153
30	BEND	12	11	1				1.9010888	108.9243665
31	BEND	13	11	1				1.9062770	109.2216271
32	BEND	14	11	1				1.7766413	101.7940506
33	TORSION	13	11	1	12			2.3265031	133.2988075
34	TORSION	14	11	1	12			-2.0145840	-115.4271611
35	BEND	15	14	11				1.9524269	111.8658213
36	TORSION	8	7	2	1			-0.9475677	-54.2916275
37	TORSION	11	1	2	7			3.0711472	175.9637739

38	TORSION	14	11	1	2	3.1395624	179.8836744
39	TORSION	15	14	11	1	1.5890379	91.0451626

TOTAL ENERGY DISTRIBUTION MATRIX M (VIBR. CONTRIBUTIONS SUM TO 100 %)

						1	2	3	4
						0.39206E-04	0.19607E-04	0.10005E-04	0.12444E-04
						I	I	I	
STR.	2	1				0.00000000	0.00000000	0.00000000	0.00000000
STR.	3	1				0.00000000	0.00000000	0.00000000	0.00000000
STR.	4	1				0.00000000	0.00000000	0.00000000	0.00000000
STR.	5	2				0.00000000	0.00000000	0.00000000	0.00000000
STR.	6	2				0.00000000	0.00000000	0.00000000	0.00000000
STR.	7	2				0.00000000	0.00000000	0.00000000	0.00000000
STR.	8	7				0.00000000	0.00000000	0.00000000	0.00000000
STR.	9	7				0.00000000	0.00000000	0.00000000	0.00000000
STR.	10	7				0.00000000	0.00000000	0.00000000	0.00000000
STR.	11	1				0.00000000	0.00000000	0.00000000	0.00000000
STR.	12	11				0.00000000	0.00000000	0.00000000	0.00000000
STR.	13	11				0.00000000	0.00000000	0.00000000	0.00000000
STR.	14	11				0.00000000	0.00000000	0.00000000	0.00000000
STR.	15	14				0.00000000	0.00000000	0.00000000	0.00000000
BEND	11	1	2			0.00000000	0.00000000	0.00000000	0.00000000
BEND	3	1	2			0.00000000	0.00000000	0.00000000	0.00000000
BEND	4	1	2			0.00000000	0.00000000	0.00000000	0.00000000
TORS	3	1	2	11		0.00000000	0.00000000	0.00000000	0.00000000
TORS	4	1	2	11		0.00000000	0.00000000	0.00000000	0.00000000
BEND	7	2	1			0.00000000	0.00000000	0.00000000	0.00000000
BEND	5	2	1			0.00000000	0.00000000	0.00000000	0.00000000
BEND	6	2	1			0.00000000	0.00000000	0.00000000	0.00000000
TORS	5	2	1	7		0.00000000	0.00000000	0.00000000	0.00000000
TORS	6	2	1	7		0.00000000	0.00000000	0.00000000	0.00000000
BEND	8	7	2			0.00000000	0.00000000	0.00000000	0.00000000
BEND	9	7	2			0.00000000	0.00000000	0.00000000	0.00000000
BEND	10	7	2			0.00000000	0.00000000	0.00000000	0.00000000
TORS	9	7	2	8		0.00000000	0.00000000	0.00000000	0.00000000
TORS	10	7	2	8		0.00000000	0.00000000	0.00000000	0.00000000
BEND	12	11	1			0.00000000	0.00000000	0.00000000	0.00000000
BEND	13	11	1			0.00000000	0.00000000	0.00000000	0.00000000
BEND	14	11	1			0.00000000	0.00000000	0.00000000	0.00000000
TORS	13	11	1	12		0.00000000	0.00000000	0.00000000	0.00000000
TORS	14	11	1	12		0.00000000	0.00000000	0.00000000	0.00000000
BEND	15	14	11			0.00000000	0.00000000	0.00000000	0.00000000
TORS	8	7	2	1		0.00000000	0.00000000	0.00000000	0.00000000
TORS	11	1	2	7		0.00000000	0.00000000	0.00000000	0.00000000
TORS	14	11	1	2		0.00000000	0.00000000	0.00000000	0.00000000
TORS	15	14	11	1		0.00000000	0.00000000	0.00000000	0.00000000
						5	6	7	8
						0.23633E-04	0.35199E-04	167.64	174.15
STR.	2	1				0.00000000	0.00000000	0.00069508	-0.00027396
STR.	3	1				0.00000000	0.00000000	0.00000350	0.00003516
STR.	4	1				0.00000000	0.00000000	-0.00000968	-0.00012261
STR.	5	2				0.00000000	0.00000000	0.00000087	-0.00000379
STR.	6	2				0.00000000	0.00000000	0.00000690	0.00002376
STR.	7	2				0.00000000	0.00000000	0.00241578	0.00534395

STR.	8	7			0.00000000	0.00000000	0.00002374	0.000000252
STR.	9	7			0.00000000	0.00000000	0.00000116	0.00003645
STR.	10	7			0.00000000	0.00000000	0.00000162	-0.00016745
STR.	11	1			0.00000000	0.00000000	0.00633646	0.00690852
STR.	12	11			0.00000000	0.00000000	-0.00000088	-0.00049222
STR.	13	11			0.00000000	0.00000000	-0.00027205	0.00000537
STR.	14	11			0.00000000	0.00000000	-0.00063448	-0.00017516
STR.	15	14			0.00000000	0.00000000	-0.00000126	0.00002243
BEND	11	1	2		0.00000000	0.00000000	0.29476825	0.24880647
BEND	3	1	2		0.00000000	0.00000000	-0.00097472	-0.00090524
BEND	4	1	2		0.00000000	0.00000000	-0.00086822	-0.00187586
TORS	3	1	2	11	0.00000000	0.00000000	-0.00050524	-0.00566147
TORS	4	1	2	11	0.00000000	0.00000000	-0.00505322	-0.00091915
BEND	7	2	1		0.00000000	0.00000000	0.00993344	0.00410671
BEND	5	2	1		0.00000000	0.00000000	0.00003748	0.00315072
BEND	6	2	1		0.00000000	0.00000000	-0.00059707	-0.00008474
TORS	5	2	1	7	0.00000000	0.00000000	0.00019134	-0.00007841
TORS	6	2	1	7	0.00000000	0.00000000	0.00106671	0.00096048
BEND	8	7	2		0.00000000	0.00000000	-0.00059442	0.00013961
BEND	9	7	2		0.00000000	0.00000000	-0.00250375	-0.00182799
BEND	10	7	2		0.00000000	0.00000000	-0.00082189	-0.00021714
TORS	9	7	2	8	0.00000000	0.00000000	-0.00057329	-0.00046357
TORS	10	7	2	8	0.00000000	0.00000000	-0.00158322	-0.00032842
BEND	12	11	1		0.00000000	0.00000000	0.00029655	0.20616233
BEND	13	11	1		0.00000000	0.00000000	0.17908884	0.01514129
BEND	14	11	1		0.00000000	0.00000000	0.16865918	0.11170464
TORS	13	11	1	12	0.00000000	0.00000000	0.03055586	-0.01397771
TORS	14	11	1	12	0.00000000	0.00000000	-0.03258266	0.00647457
BEND	15	14	11		0.00000000	0.00000000	-0.00001062	-0.00017879
TORS	8	7	2	1	0.00000000	0.00000000	-0.00032293	-0.00229121
TORS	11	1	2	7	0.00000000	0.00000000	0.11909273	0.11352416
TORS	14	11	1	2	0.00000000	0.00000000	0.23744237	0.30943410
TORS	15	14	11	1	0.00000000	0.00000000	-0.00270825	-0.00193834

9	10	11	12
307.84	339.46	368.19	387.98

STR.	2	1			0.08144649	0.00290509	0.00173642	0.00166443
STR.	3	1			0.00000148	0.00023750	-0.00003710	0.00000924
STR.	4	1			-0.00000274	-0.00003015	-0.00003733	-0.00002847
STR.	5	2			0.00000119	-0.00005648	-0.00000067	-0.00026665
STR.	6	2			0.00000205	0.00000368	0.00029531	0.00022231
STR.	7	2			0.03906020	0.00064486	0.00033931	0.00124917
STR.	8	7			0.00000009	0.00002210	0.00005928	0.00002647
STR.	9	7			0.00011807	0.00002878	0.00017854	0.00025085
STR.	10	7			0.00001743	-0.00007677	0.00005345	-0.00032587
STR.	11	1			0.23441543	0.00371976	0.05529820	0.01509556
STR.	12	11			-0.00002758	-0.00012787	-0.00000475	-0.00026330
STR.	13	11			0.00000877	0.00010156	0.00023079	0.00029401
STR.	14	11			0.00094326	0.00004296	-0.00050809	-0.00008665
STR.	15	14			-0.00000110	-0.00014897	-0.00002398	-0.00004543
BEND	11	1	2		0.12770774	0.00226626	0.05874292	0.03909919
BEND	3	1	2		0.00078592	-0.00023178	0.00473919	0.00020666
BEND	4	1	2		0.00091881	-0.00098012	0.00288313	0.00340635
TORS	3	1	2	11	0.00010246	-0.00269581	-0.00137593	-0.00027983
TORS	4	1	2	11	0.00052428	-0.00133623	0.00092414	0.00088340
BEND	7	2	1		0.09895540	-0.00003856	0.34505275	0.11955879
BEND	5	2	1		-0.00036927	-0.00017853	0.01146513	-0.00087572
BEND	6	2	1		-0.00082902	0.00012424	0.00036310	0.00098563

TORS	5	2	1	7	-0.00078699	-0.00166927	-0.00659693	-0.00065898
TORS	6	2	1	7	-0.00008431	0.00196672	0.01746090	0.00532672
BEND	8	7	2		0.00003500	-0.00125682	-0.00842886	-0.00086864
BEND	9	7	2		-0.00038803	0.00001890	-0.00242200	-0.00142287
BEND	10	7	2		0.00062713	-0.00262030	0.00278468	-0.00864651
TORS	9	7	2	8	-0.00007233	-0.00116766	-0.00138345	-0.00189995
TORS	10	7	2	8	0.00043737	0.00007058	-0.00274315	0.00043422
BEND	12	11	1		-0.00925722	0.09154420	0.11074989	0.03754561
BEND	13	11	1		0.01161324	0.11323574	0.02867779	-0.00391513
BEND	14	11	1		0.38719526	0.01249922	0.08916046	0.03799769
TORS	13	11	1	12	0.02399436	-0.01643455	0.00274435	0.02014595
TORS	14	11	1	12	0.00280443	0.32881654	-0.00571487	0.00079816
BEND	15	14	11		0.00054018	0.01730612	0.00223561	0.00782553
TORS	8	7	2	1	0.00006535	0.00169464	-0.00454102	0.02149537
TORS	11	1	2	7	0.00234251	0.23323697	0.13584638	0.44465292
TORS	14	11	1	2	-0.00053219	-0.01679202	0.13571310	0.18586454
TORS	15	14	11	1	-0.00231312	0.23535545	0.02608329	0.07454523

13	14	15	16
434.77	498.23	499.48	575.71

STR.	2	1			0.00185973	0.00515919	-0.00000869	0.02452722
STR.	3	1			0.00055972	0.00004793	0.00013492	0.00002273
STR.	4	1			-0.00025046	-0.00000064	-0.00004664	0.00001110
STR.	5	2			-0.00001334	-0.00002836	-0.00000015	0.00000090
STR.	6	2			0.00009458	-0.00002808	0.00000452	0.00000340
STR.	7	2			0.00100173	0.00011713	0.00001323	0.02788420
STR.	8	7			-0.00000033	0.00000156	0.00000020	-0.00000042
STR.	9	7			0.00000464	0.00003749	0.00000414	0.00007549
STR.	10	7			-0.00000177	-0.00001679	0.00000033	0.00001364
STR.	11	1			0.00010771	0.00937214	0.00064765	0.00454695
STR.	12	11			0.00030191	0.00164884	0.00725380	0.00110220
STR.	13	11			0.00096626	0.00354937	0.00089146	0.00279684
STR.	14	11			0.00194534	0.03868580	0.00069346	0.04667005
STR.	15	14			0.00003516	0.00004850	0.00048505	0.00014921
BEND	11	1	2		0.00084058	0.01790539	0.00029867	0.06595174
BEND	3	1	2		-0.00211861	0.00107605	0.00028926	-0.00120059
BEND	4	1	2		-0.00610972	0.00071424	0.00000247	-0.00143830
TORS	3	1	2	11	-0.00761706	-0.00111911	-0.00107801	-0.00299422
TORS	4	1	2	11	0.00069236	0.00020280	0.00264626	-0.00218965
BEND	7	2	1		0.00533744	0.07005363	0.00399617	0.09306770
BEND	5	2	1		0.00296619	0.00067423	0.00070317	-0.00039807
BEND	6	2	1		0.00008450	0.00211515	-0.00004307	-0.00058940
TORS	5	2	1	7	0.00185028	0.00048294	0.00017210	-0.00060988
TORS	6	2	1	7	0.00676465	-0.00081225	0.00073611	-0.00020126
BEND	8	7	2		0.00005077	-0.00017776	-0.00001376	0.00030524
BEND	9	7	2		-0.00006334	-0.00066425	0.00001171	0.00000613
BEND	10	7	2		-0.00048616	0.00019908	0.00008231	0.00059230
TORS	9	7	2	8	-0.00004249	0.00031611	0.00005193	0.00019738
TORS	10	7	2	8	-0.00002146	-0.00004470	0.00004828	0.00062805
BEND	12	11	1		0.19477824	0.04093777	-0.02346082	0.28952803
BEND	13	11	1		0.29101669	-0.01500026	0.03113542	0.29085183
BEND	14	11	1		0.00391807	0.02522556	-0.00738282	0.08743724
TORS	13	11	1	12	0.04217656	0.65504010	0.12634734	0.06908412
TORS	14	11	1	12	0.06459239	0.12446424	0.46502401	-0.00625969
BEND	15	14	11		0.00342990	0.00242493	0.00571439	-0.00038268
TORS	8	7	2	1	-0.00078541	0.00284049	-0.00064389	0.00023232
TORS	11	1	2	7	-0.03139435	-0.00304488	-0.00354121	0.00016213
TORS	14	11	1	2	0.18765607	0.00547204	-0.02044978	0.00275349

TORS	15	14	11	1	0.23587304	0.01212437	0.40928048	0.00766251
					17	18	19	20
					760.93	782.20	831.98	952.22
STR.	2	1			0.00201848	0.01849126	0.00020713	0.02467141
STR.	3	1			-0.00003594	0.00005293	0.00001630	-0.00008692
STR.	4	1			-0.00005244	-0.00000158	0.00002483	0.00011325
STR.	5	2			0.00001464	0.00000480	0.00000010	0.00025219
STR.	6	2			0.00001470	-0.00002582	-0.00000702	-0.00066388
STR.	7	2			0.00158295	0.06142878	0.00026594	-0.00204744
STR.	8	7			0.00001502	0.00003106	-0.00000139	0.00004204
STR.	9	7			0.00026237	-0.00076126	-0.00001043	-0.00004457
STR.	10	7			0.00046384	0.00064827	0.00001448	0.00004398
STR.	11	1			0.41665487	0.10506418	0.10796444	0.00739408
STR.	12	11			0.01933386	0.00719764	0.00081298	0.00000071
STR.	13	11			0.01586938	0.00594295	0.00026615	0.00044272
STR.	14	11			0.05932519	0.07691488	0.75760552	0.00053705
STR.	15	14			0.00001898	0.00004441	0.00014864	0.00000242
BEND	11	1	2		0.08036765	0.00481189	-0.00004757	0.00301634
BEND	3	1	2		-0.00155690	0.00522826	0.00480175	0.12220264
BEND	4	1	2		-0.00294110	-0.00030361	0.00189649	0.10159667
TORS	3	1	2	11	-0.00911420	-0.00068892	-0.00114055	0.04593570
TORS	4	1	2	11	-0.00282036	0.00227705	0.00954613	0.04439111
BEND	7	2	1		0.07345604	0.03512456	0.01162222	-0.00098348
BEND	5	2	1		-0.00137261	0.00157657	0.00024754	0.18746745
BEND	6	2	1		-0.00033129	0.00322988	0.00119581	0.09265592
TORS	5	2	1	7	0.00094059	0.01699880	0.00119137	0.09020078
TORS	6	2	1	7	0.00224774	0.02495372	0.00129677	0.22646835
BEND	8	7	2		-0.00035775	0.00995921	0.00045655	0.00101698
BEND	9	7	2		0.01581705	0.02238777	-0.00005963	0.00466083
BEND	10	7	2		0.04045829	0.07053739	0.00084095	-0.00028806
TORS	9	7	2	8	0.06643054	0.16220972	0.00298882	0.00967901
TORS	10	7	2	8	0.04138416	0.07070792	0.00046219	0.00833651
BEND	12	11	1		0.01023981	0.00204606	0.02336312	-0.00083758
BEND	13	11	1		0.01343513	0.00179633	0.02981887	-0.00019155
BEND	14	11	1		0.04340073	0.00329381	-0.00196227	0.00055402
TORS	13	11	1	12	-0.00084609	0.01175212	0.02515289	-0.00227757
TORS	14	11	1	12	0.01098781	-0.01033465	0.00831687	0.00097545
BEND	15	14	11		-0.00065383	0.00038170	0.00287040	-0.00002481
TORS	8	7	2	1	0.10394238	0.29720720	0.00808341	-0.00594335
TORS	11	1	2	7	0.00440355	0.00604533	-0.00056872	0.01201688
TORS	14	11	1	2	-0.00258983	-0.01633832	0.00020638	0.02875928
TORS	15	14	11	1	-0.00041340	0.00010770	0.00211253	-0.00004456
					21	22	23	24
					988.54	1043.7	1124.0	1135.5
STR.	2	1			0.05375201	0.68535607	0.02513177	0.04339853
STR.	3	1			0.00000147	-0.00028632	-0.00028673	-0.00047947
STR.	4	1			-0.00002175	0.00014567	0.00019255	0.00040667
STR.	5	2			0.00014925	0.00015309	0.00004956	0.00012835
STR.	6	2			0.00012856	0.00008649	-0.00001142	-0.00000807
STR.	7	2			0.71670075	0.11226354	0.01004770	0.02170762
STR.	8	7			-0.00017897	-0.00000657	0.00003526	0.00008818
STR.	9	7			0.00022747	-0.00000977	-0.00000764	-0.00001639
STR.	10	7			0.00008846	0.00004858	-0.00000148	-0.00000286
STR.	11	1			0.00068545	0.00168219	0.00274010	0.00006542
STR.	12	11			0.00137260	-0.00001982	-0.00002614	0.00357327

STR.	13	11		0.00048430	0.00172695	0.02463405	0.06008713
STR.	14	11		0.00089596	0.00306480	0.00014082	-0.00392195
STR.	15	14		-0.00000196	0.00000244	-0.00050489	-0.00022425
BEND	11	1	2	0.04829124	-0.00956978	0.00167337	0.00212762
BEND	3	1	2	-0.00001014	0.05649948	0.01753087	0.06267663
BEND	4	1	2	0.00118906	0.00149705	-0.00004207	0.00072609
TORS	3	1	2 11	-0.00047536	0.01529340	0.03897782	0.05353998
TORS	4	1	2 11	-0.00058903	0.04530789	0.15080710	0.22731235
BEND	7	2	1	0.11928333	0.02837987	0.00128240	0.00150690
BEND	5	2	1	-0.00321673	0.01739201	0.00366307	0.00331289
BEND	6	2	1	-0.00142391	-0.00005455	-0.00158925	0.00027518
TORS	5	2	1 7	-0.00560182	0.00662770	0.00836652	0.02157019
TORS	6	2	1 7	-0.01423801	0.00278727	0.06934982	0.17267832
BEND	8	7	2	-0.00210889	0.00982910	0.00508708	0.01358781
BEND	9	7	2	-0.00078556	0.00293183	0.00154806	0.00302193
BEND	10	7	2	-0.00152143	-0.00103713	-0.00051810	0.00010578
TORS	9	7	2 8	0.00643925	0.00113380	0.00007263	0.00011743
TORS	10	7	2 8	-0.00356082	-0.00001924	0.00207550	0.00407473
BEND	12	11	1	0.00485594	-0.00062046	0.01099225	0.00651426
BEND	13	11	1	0.00058476	0.00234854	0.00080575	0.00451981
BEND	14	11	1	0.00761450	0.01802827	-0.00043995	0.00432200
TORS	13	11	1 12	0.01280529	0.00481731	-0.00304299	0.00401501
TORS	14	11	1 12	-0.00622935	-0.00295383	0.01662165	0.01203781
BEND	15	14	11	0.00035147	0.00018760	0.61579794	0.27998721
TORS	8	7	2 1	0.06132471	0.00223432	-0.00609033	-0.01281604
TORS	11	1	2 7	0.00206546	-0.00056124	0.00083131	0.00340862
TORS	14	11	1 2	0.00066202	-0.00500320	0.00011708	0.00696042
TORS	15	14	11 1	0.00001042	0.00031664	0.00398896	-0.00038512

25
1175.2

26
1208.5

27
1320.6

28
1357.4

STR.	2	1		0.00018294	0.00283029	0.00009460	0.00164345
STR.	3	1		-0.00001449	-0.00007356	0.00000328	-0.00035592
STR.	4	1		-0.00000952	0.00002633	-0.00003588	0.00023791
STR.	5	2		-0.00000489	0.00010326	0.00016902	0.00005865
STR.	6	2		0.00001630	0.00013152	0.00000140	-0.00007803
STR.	7	2		0.00013023	0.00514048	0.01460789	0.00167119
STR.	8	7		0.00000030	0.00011501	0.00015140	-0.00001378
STR.	9	7		-0.00000288	-0.00000043	-0.00010471	-0.00007598
STR.	10	7		0.00000244	0.00004430	0.00083337	0.00035698
STR.	11	1		0.01594832	0.00392045	0.00192112	0.00005128
STR.	12	11		0.50585149	0.04568831	0.04461584	0.14337355
STR.	13	11		0.38402379	0.00076839	0.03181944	0.18865793
STR.	14	11		0.01807775	-0.00002045	-0.00009107	-0.00002811
STR.	15	14		-0.00003831	-0.00001118	-0.00000267	-0.00001162
BEND	11	1	2	0.00507193	-0.00248098	0.02345073	0.00558410
BEND	3	1	2	0.00143522	0.02027451	0.07634972	0.05177093
BEND	4	1	2	0.01022313	0.24299930	0.05711989	0.06466849
TORS	3	1	2 11	0.00048331	0.00292328	-0.00311678	0.02498729
TORS	4	1	2 11	0.00232600	0.20941989	0.02820107	0.00921456
BEND	7	2	1	0.00062198	0.00374423	-0.02938171	-0.00807830
BEND	5	2	1	0.00254050	0.10809742	0.14152465	0.13294087
BEND	6	2	1	0.00025259	0.03251811	0.01614050	0.14035173
TORS	5	2	1 7	0.00196173	0.04897015	0.02786207	0.00059863
TORS	6	2	1 7	0.00652239	0.13981743	0.00493480	0.01821476
BEND	8	7	2	0.00250374	0.01851204	0.03668430	0.05417893
BEND	9	7	2	0.00108259	0.00303370	0.19470565	0.08335663
BEND	10	7	2	-0.00001620	0.04675502	0.15489233	0.02257482

TORS	9	7	2	8	-0.00004053	-0.00699108	-0.04196614	-0.00867756
TORS	10	7	2	8	0.00073459	-0.00935429	0.02809417	0.02580074
BEND	12	11	1		0.00156085	0.00249560	-0.00327307	0.00093107
BEND	13	11	1		0.00232742	0.00008635	-0.00165310	0.00090323
BEND	14	11	1		0.00705757	0.00022791	-0.00015605	-0.00006925
TORS	13	11	1	12	0.00821935	-0.00037512	-0.00162001	-0.00074773
TORS	14	11	1	12	0.00433668	-0.00004253	-0.00641295	0.00989173
BEND	15	14	11		0.01585743	0.00295772	0.00110455	0.01570879
TORS	8	7	2	1	-0.00021250	0.05957968	0.20606358	0.02282334
TORS	11	1	2	7	0.00050073	0.01570282	0.00116687	-0.00281700
TORS	14	11	1	2	0.00004774	0.00240798	-0.00479919	0.00047478
TORS	15	14	11	1	0.00043830	0.00005814	0.00010109	-0.00007310

29	30	31	32
1372.6	1459.4	1512.4	1540.7

STR.	2	1			0.00246932	0.00383173	0.00093913	0.01427644
STR.	3	1			-0.00003503	-0.00018737	-0.00010111	-0.00027484
STR.	4	1			0.00038389	0.00006711	0.00016977	-0.00008635
STR.	5	2			0.00014963	0.00076889	-0.00002946	0.00002642
STR.	6	2			-0.00010635	-0.00006593	0.00042687	-0.00001588
STR.	7	2			0.00009506	-0.00927254	0.00061002	-0.00083132
STR.	8	7			-0.00000995	-0.00012361	-0.00012801	0.00004492
STR.	9	7			-0.00000880	-0.00013380	0.00001675	-0.00002244
STR.	10	7			0.00001322	0.00178354	0.00015155	-0.00002244
STR.	11	1			0.00061527	0.00030056	0.00106958	0.00034216
STR.	12	11			0.21441940	0.00234554	0.00070569	0.00093869
STR.	13	11			0.27648799	-0.00001209	-0.00002079	0.00043669
STR.	14	11			-0.00039302	0.00003058	0.00006173	0.00001704
STR.	15	14			-0.00001842	-0.00000080	-0.00000010	-0.00000194
BEND	11	1	2		-0.00105320	0.00194371	-0.00165126	0.00030008
BEND	3	1	2		0.03817794	0.01578043	0.08244780	0.40090680
BEND	4	1	2		0.17775344	0.03764705	0.05927244	0.22543328
TORS	3	1	2	11	0.00849352	0.00882294	0.00121014	0.00138944
TORS	4	1	2	11	0.02050589	0.01491181	0.03396970	0.09058730
BEND	7	2	1		-0.00021760	0.01522464	0.00536318	-0.00181475
BEND	5	2	1		0.13474168	0.16424363	-0.00138253	0.02331309
BEND	6	2	1		0.06447737	0.16905431	0.07263316	0.10503856
TORS	5	2	1	7	-0.00096378	0.19259742	0.03311329	0.05211116
TORS	6	2	1	7	0.00201768	-0.00046974	0.15298071	0.03884586
BEND	8	7	2		0.01689523	0.08492176	0.38348007	0.03735958
BEND	9	7	2		0.00655976	0.00115452	0.06965064	-0.00007028
BEND	10	7	2		0.00033786	0.24602166	0.06373986	0.00042107
TORS	9	7	2	8	0.00102302	-0.02383823	0.00825887	0.00153092
TORS	10	7	2	8	0.00364346	-0.00726526	0.03495523	0.00691236
BEND	12	11	1		0.00358004	-0.00070487	0.00000256	0.00039086
BEND	13	11	1		0.00088365	-0.00082644	0.00183201	0.00075275
BEND	14	11	1		0.00005675	-0.00013253	0.00044573	0.00106078
TORS	13	11	1	12	0.00058782	0.00128287	-0.00027256	0.00110888
TORS	14	11	1	12	0.02129295	-0.00523267	0.00099171	-0.00194549
BEND	15	14	11		0.02605602	0.00007867	0.00008945	0.00033449
TORS	8	7	2	1	-0.00010995	0.12985342	0.01211123	0.00021109
TORS	11	1	2	7	-0.00281371	-0.02136372	-0.01685355	-0.00002795
TORS	14	11	1	2	-0.01580089	-0.02297529	-0.00025218	0.00103200
TORS	15	14	11	1	-0.00018712	-0.00006190	-0.00000729	-0.00000901

33	34	35	36
1603.6	1664.2	1780.8	1845.6

STR.	2	1			-0.00066256	0.00118982	-0.00044995	0.00003389
STR.	3	1			-0.00000364	0.00000049	0.00541115	0.00000663
STR.	4	1			-0.00000166	0.00000382	-0.00037814	-0.00000109
STR.	5	2			-0.00024794	-0.00000848	0.00000456	0.00002686
STR.	6	2			0.00033896	0.00000003	0.00002305	0.00001949
STR.	7	2			-0.00129015	-0.00671543	-0.00027134	-0.00251967
STR.	8	7			-0.00004060	-0.00002469	0.00000831	-0.00080043
STR.	9	7			0.00000035	0.00045745	0.00000690	0.00001825
STR.	10	7			0.00005739	-0.00068660	-0.00000051	-0.00010262
STR.	11	1			0.00001008	-0.00002460	-0.00271934	-0.00006221
STR.	12	11			0.00001845	0.00000002	0.00038819	0.00000485
STR.	13	11			0.00001846	-0.00000015	-0.00023464	-0.00000329
STR.	14	11			0.00000062	-0.00000053	0.00012899	-0.00000122
STR.	15	14			0.00000003	0.00000026	-0.00000112	-0.00000012
BEND	11	1	2		0.00024031	-0.00024154	-0.01656881	-0.00058975
BEND	3	1	2		0.00016681	0.00102104	0.04082833	0.00111761
BEND	4	1	2		0.00092548	0.00065908	0.02135535	0.00002152
TORS	3	1	2	11	0.00200867	0.00001776	0.82715922	0.00461049
TORS	4	1	2	11	-0.00000093	0.00012221	0.11691547	0.00044035
BEND	7	2	1		-0.00460155	-0.00001567	-0.00155278	0.00040958
BEND	5	2	1		0.06345149	0.00286735	0.00095469	-0.00000669
BEND	6	2	1		0.29638658	0.00363036	0.00451004	0.00006377
TORS	5	2	1	7	0.50596272	0.00200876	-0.00015228	0.00049057
TORS	6	2	1	7	0.11959927	-0.00019274	-0.00012219	0.00027983
BEND	8	7	2		0.01236540	0.05480084	-0.00000694	0.20187019
BEND	9	7	2		0.00216928	0.40998591	0.00252790	0.17651333
BEND	10	7	2		0.00283845	0.14783496	-0.00001255	0.01455183
TORS	9	7	2	8	0.00249244	0.23673632	0.00518878	0.56039101
TORS	10	7	2	8	0.00012808	0.11980404	-0.00049836	-0.04966310
BEND	12	11	1		0.00006347	-0.00002617	-0.00052223	-0.00001067
BEND	13	11	1		0.00014540	0.00001247	0.00029003	-0.00004044
BEND	14	11	1		0.00000070	-0.00003249	0.00016181	-0.00001621
TORS	13	11	1	12	-0.00001251	-0.00014590	0.00009613	0.00006093
TORS	14	11	1	12	0.00007811	0.00010945	-0.00089517	-0.00019213
BEND	15	14	11		0.00000009	-0.00000007	0.00026153	-0.00000205
TORS	8	7	2	1	0.00258352	0.02999744	0.00073362	0.09533484
TORS	11	1	2	7	-0.00489814	-0.00240515	-0.00212449	-0.00294611
TORS	14	11	1	2	-0.00029471	-0.00073977	-0.00038405	0.00069348
TORS	15	14	11	1	0.00000379	0.00000010	-0.00005914	-0.00000150

37	38	39	40
2029.5	3088.9	3105.0	3144.2

STR.	2	1			0.00003929	0.00075908	0.00007247	-0.00000477
STR.	3	1			0.00001080	0.32484260	0.02124436	0.46642948
STR.	4	1			0.00000018	0.59042019	0.06088477	0.24067419
STR.	5	2			0.00005480	0.04489444	0.46153227	0.15581082
STR.	6	2			0.00000890	0.03632799	0.45565379	0.13440088
STR.	7	2			-0.00199998	-0.00005063	0.00017253	0.00000130
STR.	8	7			0.00131245	0.00002851	0.00018883	0.00013487
STR.	9	7			-0.00009456	0.00000137	-0.00000008	0.00000089
STR.	10	7			-0.00016599	0.00002909	0.00015212	0.00020928
STR.	11	1			-0.00000648	-0.00002581	-0.00002046	-0.00001540
STR.	12	11			0.00000255	0.00000059	0.00000117	0.00000372
STR.	13	11			-0.00000002	0.00000007	0.00000061	0.00000312
STR.	14	11			0.00000092	0.00000366	-0.00000013	-0.00000001
STR.	15	14			-0.00000006	-0.00000005	0.00000090	0.00000000
BEND	11	1	2		0.00003283	-0.00108804	0.00013294	-0.00007677
BEND	3	1	2		0.00000952	-0.00011079	-0.00001898	0.00079768

BEND	4	1	2		0.00007450	0.00036445	-0.00001909	0.00123408
TORS	3	1	2	11	0.00092703	0.00414740	0.00022489	-0.00323262
TORS	4	1	2	11	0.00010621	-0.00032222	0.00003245	0.00070358
BEND	7	2	1		-0.00007436	0.00014201	0.00031532	-0.00003693
BEND	5	2	1		0.00006848	0.00015801	-0.00010469	0.00041725
BEND	6	2	1		-0.00000241	-0.00000029	0.00009308	-0.00029054
TORS	5	2	1	7	0.00097752	-0.00007480	-0.00064490	0.00102311
TORS	6	2	1	7	0.00003604	-0.00010996	-0.00021436	-0.00053560
BEND	8	7	2		0.06983255	0.00000217	0.00013217	0.00003277
BEND	9	7	2		0.00972431	0.00003015	0.00012273	-0.00000091
BEND	10	7	2		0.19540514	0.00000022	0.00010502	0.00008525
TORS	9	7	2	8	0.02474788	-0.00000165	-0.00001294	-0.00000867
TORS	10	7	2	8	0.72378266	0.00000172	-0.00000084	-0.00000129
BEND	12	11	1		-0.00000125	-0.00007334	0.00001808	0.00015943
BEND	13	11	1		0.00002189	0.00003433	0.00000004	0.00022951
BEND	14	11	1		-0.00000036	0.00017198	-0.00001799	0.00001352
TORS	13	11	1	12	-0.00001649	-0.00022945	0.00000687	-0.00001195
TORS	14	11	1	12	0.00003160	0.00015486	-0.00000591	0.00011798
BEND	15	14	11		0.00000001	0.00000002	0.00000000	-0.00000013
TORS	8	7	2	1	-0.02528574	-0.00001465	0.00000391	0.00002303
TORS	11	1	2	7	0.00046894	-0.00002986	-0.00008941	0.00007684
TORS	14	11	1	2	-0.00002964	-0.00037954	0.00005824	0.00159274
TORS	15	14	11	1	0.00000030	-0.00000383	0.00000019	0.00004027

41	42	43	44
3162.0	3404.7	3470.1	3488.1

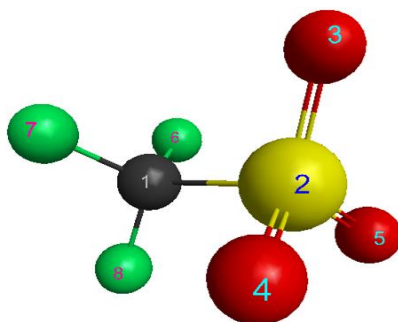
STR.	2	1			0.00000638	0.00000351	0.00000218	0.00000475
STR.	3	1			0.18318199	0.00000344	0.00000106	0.00000001
STR.	4	1			0.10735328	0.00000121	0.00000008	0.00000010
STR.	5	2			0.33549579	0.00035010	0.00045899	0.00000033
STR.	6	2			0.37209552	0.00005109	0.00049859	0.00012976
STR.	7	2			0.00000107	0.00057033	-0.00010599	0.00003750
STR.	8	7			0.00025029	0.31269558	0.44072052	0.24532972
STR.	9	7			0.00000010	0.13370028	0.11551317	0.75035095
STR.	10	7			0.00045612	0.55099651	0.44237513	0.00271562
STR.	11	1			-0.00000269	-0.00000092	0.00000017	-0.00000031
STR.	12	11			0.00000406	0.00000025	0.00000000	0.00000003
STR.	13	11			0.00000273	0.00000002	0.00000001	0.00000002
STR.	14	11			0.00000003	0.00000008	0.00000002	0.00000001
STR.	15	14			0.00000002	0.00000213	0.00000025	0.00000098
BEND	11	1	2		-0.00006213	-0.00001148	0.00000603	0.00000149
BEND	3	1	2		0.00000189	0.00000051	0.00000385	0.00000017
BEND	4	1	2		-0.00000356	0.00000000	-0.00000012	-0.00000006
TORS	3	1	2	11	-0.00016171	0.00000248	-0.00000027	-0.00000016
TORS	4	1	2	11	0.00025962	0.00000012	-0.00000030	-0.00000002
BEND	7	2	1		0.00000239	-0.00013831	-0.00008130	0.00047425
BEND	5	2	1		-0.00009901	0.00001650	0.00000738	0.00000442
BEND	6	2	1		-0.00036756	0.00000072	0.00002255	0.00000022
TORS	5	2	1	7	0.00152944	0.00004599	-0.00000015	-0.00000700
TORS	6	2	1	7	-0.00049734	-0.00001222	0.00014662	0.00003032
BEND	8	7	2		0.00029720	-0.00007033	-0.00003762	-0.00041454
BEND	9	7	2		-0.00000023	-0.00042112	-0.00002576	-0.00036578
BEND	10	7	2		0.00028301	0.00064238	0.00354658	-0.00007795
TORS	9	7	2	8	-0.00006933	0.00054079	-0.00297620	-0.00036155
TORS	10	7	2	8	0.00000339	0.00198239	0.00076647	-0.00018484
BEND	12	11	1		0.00003155	-0.00000018	0.00000007	0.00000010
BEND	13	11	1		0.00003483	0.00000004	-0.00000007	-0.00000022
BEND	14	11	1		0.00000571	0.00000132	-0.00000001	-0.00000018

TORS	13	11	1	12	0.00000032	0.00000021	0.00000000	0.00000042
TORS	14	11	1	12	0.00000880	-0.00000013	-0.00000032	-0.00000026
BEND	15	14	11		-0.00000003	0.00000002	0.00000000	0.00000004
TORS	8	7	2	1	-0.00006069	-0.00074581	-0.00082946	0.00225405
TORS	11	1	2	7	0.00003670	-0.00020549	0.00001083	0.00009182
TORS	14	11	1	2	-0.00002980	-0.00000201	-0.00002294	-0.00001419
TORS	15	14	11	1	0.00001186	0.00000000	-0.00000001	-0.00000001

45
3732.0

STR.	2	1			0.00000035
STR.	3	1			0.00000026
STR.	4	1			0.00000021
STR.	5	2			0.00000045
STR.	6	2			0.00000010
STR.	7	2			0.00000004
STR.	8	7			0.00000055
STR.	9	7			0.00000184
STR.	10	7			0.00000038
STR.	11	1			0.00000013
STR.	12	11			0.00000236
STR.	13	11			0.00002573
STR.	14	11			0.00007437
STR.	15	14			1.00007641
BEND	11	1	2		0.00000184
BEND	3	1	2		0.00000029
BEND	4	1	2		0.00000001
TORS	3	1	2	11	0.00000007
TORS	4	1	2	11	-0.00000001
BEND	7	2	1		0.00000036
BEND	5	2	1		0.00000001
BEND	6	2	1		0.00000002
TORS	5	2	1	7	0.00000002
TORS	6	2	1	7	-0.00000002
BEND	8	7	2		0.00000004
BEND	9	7	2		0.00000018
BEND	10	7	2		0.00000002
TORS	9	7	2	8	-0.00000004
TORS	10	7	2	8	0.00000018
BEND	12	11	1		0.00000012
BEND	13	11	1		0.00000324
BEND	14	11	1		-0.00000434
TORS	13	11	1	12	0.00001557
TORS	14	11	1	12	-0.00012518
BEND	15	14	11		-0.00024881
TORS	8	7	2	1	0.00000004
TORS	11	1	2	7	0.00000046
TORS	14	11	1	2	0.00008169
TORS	15	14	11	1	0.00009106

S6. DFT calculations of TfO⁻



NO.	TYPE	- - ATOMS - -						COORDINATE (BOHR, RAD)	COORDINATE (ANG, DEG)
		I	J	K	L	M	N		
1	STRETCH	2	1					3.5260068	1.8658826
2	STRETCH	3	2					2.7488076	1.4546064
3	STRETCH	4	2					2.7488169	1.4546113
4	STRETCH	5	2					2.7489988	1.4547076
5	STRETCH	6	1					2.5365870	1.3423041
6	STRETCH	7	1					2.5343993	1.3411464
7	STRETCH	8	1					2.5365710	1.3422956
8	BEND	3	2	1				1.8019730	103.2454468
9	BEND	4	2	1				1.8019874	103.2462740
10	BEND	5	2	1				1.7986953	103.0576492
11	BEND	6	1	2				1.9386144	111.0744227
12	BEND	7	1	2				1.9415101	111.2403355
13	BEND	8	1	2				1.9386502	111.0764719
14	TORSION	3	2	1	4			-2.0958142	-120.0813106
15	TORSION	3	2	1	5			2.0937023	119.9603032
16	TORSION	7	1	2	6			-2.0955947	-120.0687340
17	TORSION	7	1	2	8			2.0956650	120.0727591
18	TORSION	3	2	1	7			-1.0475598	-60.0207579

TOTAL ENERGY DISTRIBUTION MATRIX M (VIBR. CONTRIBUTIONS SUM TO 100 %)

					1	2	3	4
					0.16585E-04	0.14340E-04	0.11053E-04	0.72465E-05
					I	I	I	I
STR.	2	1			0.00000000	0.00000000	0.00000000	0.00000000
STR.	3	2			0.00000000	0.00000000	0.00000000	0.00000000
STR.	4	2			0.00000000	0.00000000	0.00000000	0.00000000
STR.	5	2			0.00000000	0.00000000	0.00000000	0.00000000
STR.	6	1			0.00000000	0.00000000	0.00000000	0.00000000
STR.	7	1			0.00000000	0.00000000	0.00000000	0.00000000
STR.	8	1			0.00000000	0.00000000	0.00000000	0.00000000
BEND	3	2	1		0.00000000	0.00000000	0.00000000	0.00000000
BEND	4	2	1		0.00000000	0.00000000	0.00000000	0.00000000
BEND	5	2	1		0.00000000	0.00000000	0.00000000	0.00000000
BEND	6	1	2		0.00000000	0.00000000	0.00000000	0.00000000
BEND	7	1	2		0.00000000	0.00000000	0.00000000	0.00000000
BEND	8	1	2		0.00000000	0.00000000	0.00000000	0.00000000
TORS	3	2	1	4	0.00000000	0.00000000	0.00000000	0.00000000
TORS	3	2	1	5	0.00000000	0.00000000	0.00000000	0.00000000
TORS	7	1	2	6	0.00000000	0.00000000	0.00000000	0.00000000
TORS	7	1	2	8	0.00000000	0.00000000	0.00000000	0.00000000

TORS	3	2	1	7	0.00000000	0.00000000	0.00000000	0.00000000
					5	6	7	8
					0.90601E-05	0.15391E-04	69.897	190.37
STR.	2	1			0.00000000	0.00000000	0.00000000	0.00000200
STR.	3	2			0.00000000	0.00000000	0.00000173	-0.00005134
STR.	4	2			0.00000000	0.00000000	0.00000182	-0.00004763
STR.	5	2			0.00000000	0.00000000	0.00000000	-0.00037224
STR.	6	1			0.00000000	0.00000000	-0.00000005	-0.00019557
STR.	7	1			0.00000000	0.00000000	0.00000000	-0.00089520
STR.	8	1			0.00000000	0.00000000	-0.00000004	-0.00021954
BEND	3	2	1		0.00000000	0.00000000	0.00016068	0.09282777
BEND	4	2	1		0.00000000	0.00000000	0.00016315	0.08360688
BEND	5	2	1		0.00000000	0.00000000	0.00000004	0.34691985
BEND	6	1	2		0.00000000	0.00000000	0.00007707	0.07399692
BEND	7	1	2		0.00000000	0.00000000	0.00000002	0.30984887
BEND	8	1	2		0.00000000	0.00000000	0.00007592	0.08211671
TORS	3	2	1	4	0.00000000	0.00000000	0.00002761	0.00312495
TORS	3	2	1	5	0.00000000	0.00000000	-0.00611714	-0.00000534
TORS	7	1	2	6	0.00000000	0.00000000	-0.00125114	0.00483904
TORS	7	1	2	8	0.00000000	0.00000000	-0.00126305	0.00451255
TORS	3	2	1	7	0.00000000	0.00000000	1.00812339	-0.00000869
					9	10	11	12
					190.68	294.29	335.67	337.55
STR.	2	1			0.00000000	0.64499036	0.00000001	0.00000157
STR.	3	2			-0.00012233	0.00001844	0.00080811	0.00021548
STR.	4	2			-0.00012776	0.00001824	0.00080143	0.00022054
STR.	5	2			-0.00000007	0.00001033	0.00000001	0.00079139
STR.	6	1			-0.00075850	0.00173841	0.00505436	0.00170830
STR.	7	1			-0.00000020	0.00182686	0.00000009	0.00668214
STR.	8	1			-0.00073401	0.00174110	0.00508939	0.00167073
BEND	3	2	1		0.25531664	0.04839290	0.20441600	0.06667818
BEND	4	2	1		0.26443212	0.04832465	0.20301693	0.06814166
BEND	5	2	1		0.00008072	0.04851184	0.00000265	0.27725331
BEND	6	1	2		0.23929246	0.06865010	0.25771366	0.08874768
BEND	7	1	2		0.00006985	0.06700503	0.00000413	0.34597038
BEND	8	1	2		0.23116906	0.06876000	0.25962925	0.08671783
TORS	3	2	1	4	-0.00003604	0.00001184	0.00006161	0.04050493
TORS	3	2	1	5	0.00030090	0.00000005	0.04969296	0.00006880
TORS	7	1	2	6	0.00703653	-0.00000014	0.00723986	0.00726546
TORS	7	1	2	8	0.00739575	-0.00000013	0.00713161	0.00736644
TORS	3	2	1	7	-0.00331512	0.00000013	-0.00066205	-0.00000483
					13	14	15	16
					501.02	503.11	559.63	560.46
STR.	2	1			0.00000000	0.00006793	0.00000000	0.00005967
STR.	3	2			0.00429584	0.00168175	0.00551470	0.00218118
STR.	4	2			0.00427705	0.00169749	0.00557240	0.00212899
STR.	5	2			-0.00000001	0.00631758	0.00000018	0.00838986
STR.	6	1			0.01638420	0.00618510	0.06620697	0.02117313
STR.	7	1			0.00000007	0.02327993	0.00000094	0.08658328
STR.	8	1			0.01646613	0.00608473	0.06571408	0.02168806
BEND	3	2	1		-0.00173644	-0.00087260	0.02246222	0.00824925
BEND	4	2	1		-0.00170854	-0.00087713	0.02255301	0.00806309
BEND	5	2	1		-0.00000001	0.00148942	0.00000032	0.02121632

BEND	6	1	2		0.01102789	0.00220361	-0.00439664	-0.00168275
BEND	7	1	2		0.00000010	0.01505224	-0.00000009	-0.00285342
BEND	8	1	2		0.01106485	0.00217421	-0.00439793	-0.00172450
TORS	3	2	1	4	0.00064897	0.60086767	-0.00072304	0.33384093
TORS	3	2	1	5	0.62081549	0.00057230	0.31754138	-0.00067687
TORS	7	1	2	6	0.15884485	0.16613367	0.25284897	0.24870003
TORS	7	1	2	8	0.15728974	0.16794926	0.25662154	0.24463637
TORS	3	2	1	7	0.00232981	-0.00000718	-0.00551900	0.00002738

17	18	19	20
611.25	746.40	1013.8	1101.9

STR.	2	1			0.03037970	0.12894139	0.01466394	0.00000000
STR.	3	2			0.00353053	0.00325455	0.27230177	0.00143916
STR.	4	2			0.00352376	0.00325443	0.27233600	0.00145649
STR.	5	2			0.00282834	0.00314298	0.27262301	0.00000000
STR.	6	1			-0.00128935	0.16611796	0.04103840	0.41152263
STR.	7	1			-0.00166220	0.16164491	0.04145556	0.00000332
STR.	8	1			-0.00129274	0.16612205	0.04101409	0.40904402
BEND	3	2	1		0.25610259	0.01801719	-0.00003497	0.01528721
BEND	4	2	1		0.25627846	0.01802280	-0.00003296	0.01537385
BEND	5	2	1		0.25842091	0.01770091	0.00010310	0.00000016
BEND	6	1	2		0.06477463	0.10464634	0.01477724	-0.00220993
BEND	7	1	2		0.06240106	0.10448571	0.01496280	0.00000001
BEND	8	1	2		0.06480729	0.10464223	0.01478153	-0.00216922
TORS	3	2	1	4	0.00120872	0.00000892	0.00000952	-0.00000316
TORS	3	2	1	5	-0.00000444	-0.00000003	-0.00000010	0.00194659
TORS	7	1	2	6	-0.00000502	-0.00000119	0.00000041	0.07367572
TORS	7	1	2	8	-0.00000463	-0.00000118	0.00000058	0.07456154
TORS	3	2	1	7	0.00000239	0.00000004	0.00000007	0.00007160

21	22	23	24
1107.6	1197.0	1236.1	1240.2

STR.	2	1			0.00000317	0.18089030	0.00000000	-0.00000006
STR.	3	2			0.00052700	0.05435248	0.48880548	0.16124547
STR.	4	2			0.00051619	0.05433314	0.48727460	0.16276282
STR.	5	2			0.00182754	0.05450413	0.00000120	0.64993578
STR.	6	1			0.13555432	0.12555849	0.00299563	0.00100556
STR.	7	1			0.54669726	0.13037557	0.00000001	0.00400765
STR.	8	1			0.13793896	0.12566640	0.00301077	0.00099582
BEND	3	2	1		0.00505743	0.00979903	0.00009153	-0.00021460
BEND	4	2	1		0.00496042	0.00980992	0.00008761	-0.00021591
BEND	5	2	1		0.01943351	0.00968165	0.00000000	-0.00081469
BEND	6	1	2		-0.00152901	0.08182916	0.00152107	0.00056050
BEND	7	1	2		-0.00047694	0.08138344	0.00000000	0.00214681
BEND	8	1	2		-0.00154757	0.08181770	0.00152790	0.00055473
TORS	3	2	1	4	0.00219585	0.00000034	0.00001058	0.01823982
TORS	3	2	1	5	-0.00000339	0.00000000	0.01583442	0.00003442
TORS	7	1	2	6	0.07485641	-0.00000086	-0.00006731	-0.00011529
TORS	7	1	2	8	0.07398699	-0.00000091	-0.00006635	-0.00011612
TORS	3	2	1	7	0.00000187	0.00000000	-0.00102715	-0.00001268

Note: The wavenumber given in the TOTAL ENERGY DISTRIBUTION MATRIX M is unscaled.