Rearrangement of the Cyclohexadiene Derivatives of C₆₀ to Bis(fulleroid) and Bis(methano)fullerene: Structure, Stability and Mechanism

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All calculations were carried out using Hyper Chem 6.0 and GAUSSIAN 98 (Revision A.11) set of programs. Cartesian coordinates for **1c-5c** optimized at AM1 level were already reported.¹ These geometries are further optimized using PM3, RHF/6-31G* and B3LYP/6-31G* levels.

¹ Iwamatsu, S.; Vijayalakshimi, P. S.; Hamajima, M.; Suresh, C. H.; Koga, N.; Suzuki, T.; Murata, S. *Org. Lett.* **2002**, 4, 1217.
(in supporting information)

Table S1. Calculated total and relative energies for **1c-5c**.

	B3LYP	rel. to 1c	RHF	rel. to 1c
	(a.u.)	(kcal/mol)	(a.u.)	(kcal/mol)
1c	-3824.2382	0	-3800.5475	0
2c	-3824.2129	15.9	—	—
3c	-3824.2236	9.2	-3800.5274	12.6
4c	-3824.2532	-9.4	—	—
5c	-3824.2441	-3.7	—	—

Table S2. Calculated total and relative energies for the systems depicted in Figure 5.

	UAM1	rel. to m-1a	UB3LYP	rel. to m-1a
			(single point)	
	(kcal/mol)	(kcal/mol)	(a.u.)	(kcal/mol)
m-1a	321.75	—	-1227.6786	—
TS1	355.41	33.66	-1227.6191	37.36
13	349.04	27.29	-1227.6071	44.91
TS2	359.24	37.49	-1227.5928	53.84
14	341.64	19.89	-1227.5926	54.00
TS3	363.89	42.14	-1227.5874	57.25
TS4	366.51	44.76	-1227.6099	43.16
m-3a	351.77	30.02	-1227.6345	27.69
m-4a	320.38	-1.37	-1227.6567	13.75

Table S3. Calculated total and relative energies for the systems depicted in Figure 6.

	UB3LYP	rel. to 1a
	(a.u.)	(kcal/mol)
1a	-2440.9684	—
TS5	-2440.9018	41.8
3a	-2440.9441	15.2

Table S4. Calculated total and relative energies for the systems depicted in Figure 7.

	triplet	rel. to	singlet	rel. to	projected
		1 a (S₀)	(singlepoint)	1 a (S₀)	singlet
	(a.u.)	(kcal/mol)	(a.u.)	(kcal/mol)	(kcal/mol)
1 a	-2440.9099	36.73	-2440.9540	9.02	9.02
TS 6	-2440.8969	44.83	-2440.9243	27.68	27.48
1 5	-2440.9101	36.55	-2440.9090	37.26	38.00
TS 7	-2440.9012	42.14	-2440.8997	43.12	44.12
1 6	-2440.9039	40.43	-2440.9029	41.10	41.77
TS 8	-2440.8915	48.25	-2440.8952	45.92	44.78
TS 9	-2440.8616	67.00	-2440.9030	41.05	40.90
3 a	-2440.8883	50.26	-2440.9365	20.03	20.01
4 a	-2440.9279	25.41	-2440.9731	-2.95	-2.96
TS 15 to 2 a	-2440.8900	49.18	-2440.9053	39.58	39.55
2 a	-2440.8960	45.43	-2440.9247	27.40	27.38

Table S5. Bond lengths of [6,6] and [6,5] ring fusions in the modified rings of **1c-5c**.

	[6,6] bond (Å)		[6,5] bond (Å)	
	longest/	shortest	longest/	shortest
1c	1.374 ^a /	1.374 ^a	1.479/	1.436
2c	1.384/	1.379	1.476/	1.387
3c	1.403/	1.379	1.504/	1.428
4c	1.407/	1.378	1.522/	1.444
5c	1.386/	1.382	1.472/	1.439

^a All bond lengths (4 bonds) are equal.

Table S6. Bond lengths of [6,6] and [6,5] ring fusions other than the modified rings of **1c-5c**.

	[6,6] bond (Å)			[6,5] bond (Å)		
	average	longest/	shortest	average	longest/	shortest
1c	1.397	1.399/	1.394	1.451	1.456/	1.441
2c	1.397	1.406/	1.394	1.451	1.456/	1.443
3c	1.396	1.420/	1.385	1.451	1.469/	1.434
4c	1.396	1.411/	1.386	1.451	1.456/	1.438
5c	1.397	1.402/	1.394	1.451	1.456/	1.443

Figure S5. Enlarged partial structure of **3c** (a) and 1,1-dimethyl cyclopropane (b). All H atoms of 1,1-dimethyl cyclopropane are omitted for clarify.

Figure S6. Structures of **1a**, **TS5**, and **3a** (in Å) and relative energies at the UB3LYP/6-31G* level. Spin populations higher than ± 0.15 in **TS5** are shown in parenthesis.

Figure S7. Selected bond lengths and angles depicted in Figure 7.

B3LYP/6-31G(d) optimized cartesian coordinates in angstrom unit

for the systems **1c-5c** (Figure 1 and Figure 2).

1c_B3LYP

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C	1	-5.4641260	0.5664370	-2.3485690
C	2	-5.8994200	1.3405500	-1.2705330
C	3	-5.4640290	-0.8860100	-2.2483460
C	4	-6.3459220	0.6954090	-0.0473440
C	5	-4.2913700	0.9646630	-3.1021520
C	6	-5.1780000	2.5463760	-0.9046660
C	7	-5.8989510	-1.5040320	-1.0737130
C	8	-6.3456760	-0.6969840	0.0489650
C	9	-3.5965540	2.1248840	-2.7542690
C	10	-4.0498080	2.9312220	-1.6316950
C	11	-4.2908470	-1.3840170	-2.9399910
C	12	-5.8989920	1.5025960	1.0751540
C	13	-3.5599090	-0.2400700	-3.4615820
C	14	-5.1780110	2.6467620	0.5462490
C	15	-5.1773890	-2.6479670	-0.5451040
C	16	-5.8984760	-1.3419830	1.2719720
C	17	-2.1451680	2.1264100	-2.7484060
C	18	-2.8757930	3.4272580	-0.9358730
C	19	-3.5960780	-2.4851320	-2.4347940
C	20	-5.4633890	0.8847140	2.2496080
C	21	-2.1646220	-0.2385050	-3.4408120
C	22	-4.0498550	3.1287690	1.2128300
C	23	-4.0493520	-3.1296100	-1.2121460
C	24	-5.4629850	-0.5677310	2.3498280
C	25	-1.4390090	0.9645920	-3.0772110
C	26	-2.8758110	3.5235760	0.4547150
C	27	-5.1768220	-2.5475830	0.9058130
C	28	-1.7037140	2.9200180	-1.6294970
C	29	-2.1452540	-2.4855400	-2.4298370
C	30	-4.2900870	1.3830970	2.9407740
C	31	-1.4392750	-1.3804930	-2.9168080

C	32	-3.5958760	2.4844330	2.4352930
C	33	-4.0482150	-2.9320710	1.6323830
C	34	-0.5846850	2.5069210	-0.8991970
C	35	-2.8748770	-3.5240500	-0.4545070
C	36	-4.2898020	-0.9655870	3.1029380
C	37	-0.2598610	0.5796100	-2.3319180
C	38	-1.7029290	3.1178990	1.2120530
C	39	-1.7024310	-3.1180040	-1.2123240
C	40	-3.5585770	0.2393810	3.4620740
C	41	-0.2589330	-0.8965910	-2.2314840
C	42	-2.1450540	2.4852960	2.4297440
C	43	-2.8743260	-3.4277360	0.9360820
C	44	-3.5947590	-2.1255880	2.7547730
C	45	0.1694760	1.3445160	-1.2744890
C	46	-0.5853600	2.6056440	0.5456340
C	47	-0.5847540	-2.6053900	-0.5463640
C	48	-2.1632990	0.2382590	3.4407330
C	49	0.1730400	-1.5088830	-1.0803140
C	50	-1.4385250	1.3804760	2.9164310
C	51	-1.7021290	-2.9201240	1.6292300
C	52	-2.1433770	-2.1266540	2.7483210
C	53	0.9751710	0.8132910	-0.0539520
C	54	0.1729960	1.5093800	1.0792750
C	55	-0.5835330	-2.5066660	0.8984670
C	56	-1.4374560	-0.9646100	3.0768450
C	57	0.9754200	-0.8125350	0.0525860
C	58	-0.2583100	0.8969510	2.2306250
C	59	0.1703730	-1.3440010	1.2734440
C	60	-0.2587360	-0.5792500	2.3310720
C	61	2.3833900	1.4380310	-0.1297230
C	62	2.4487010	2.9354440	-0.4059810
C	63	3.5253070	0.7281840	-0.0967550
C	64	4.8144410	1.4428590	-0.4213580
O	65	2.3334890	3.6316110	0.7249900
O	66	5.5148580	0.7295190	-1.3165610
O	67	2.5603000	3.3768560	-1.5311770
C	68	2.4448540	5.1157130	0.7607050
O	69	5.1127620	2.5374310	0.0091560
C	70	6.6464460	1.3187260	-2.0750790

C	71	2.3194480	5.4111260	2.2561910	H	110	5.2857650	2.1274830	-3.5630560
C	72	1.2933900	5.7490350	-0.0250990	H	111	7.9283930	-0.4605280	3.5924200
C	73	3.8139470	5.5457240	0.2285530	H	112	6.2750670	0.1914770	3.5948650
C	74	7.0998740	0.1471970	-2.9477920	H	113	7.4219920	0.6933440	2.3381580
C	75	7.7674720	1.7718340	-1.1356110	H	114	8.6283890	-2.0837420	1.7420130
C	76	6.1107150	2.4706710	-2.9306580	H	115	8.0860480	-0.9481340	0.4961890
C	77	3.5255030	-0.7265940	0.0955890	H	116	7.4508590	-2.6067230	0.5155220
C	78	4.8147520	-1.4410380	0.4204670	H	117	5.7485610	-3.2960510	2.3085550
C	79	2.3838310	-1.4368170	0.1281500	H	118	5.2777030	-2.1305000	3.5616240
C	80	2.4497930	-2.9342750	0.4039130	H	119	6.9020030	-2.8478410	3.5822280
O	81	5.5132650	-0.7290640	1.3182740	H	120	2.3765410	-6.4890210	-2.4319670
O	82	2.3350030	-3.6300800	-0.7273210	H	121	3.1306130	-4.9256680	-2.8163290
O	83	5.1144420	-2.5345140	-0.0118360	H	122	1.3660570	-5.0435200	-2.6476340
C	84	6.6427750	-1.3197720	2.0787770	H	123	1.3618210	-6.8388460	-0.0649340
O	85	2.5615570	-3.3761040	1.5289400	H	124	0.3283370	-5.4355380	-0.3831920
C	86	2.4470700	-5.1141220	-0.7635930	H	125	1.3441030	-5.4806420	1.0788050
C	87	7.0942370	-0.1497550	2.9545210	H	126	3.9487860	-6.6160460	-0.4158140
C	88	7.7661710	-1.7717440	1.1416080	H	127	3.8989320	-5.3607910	0.8413890
C	89	6.1044410	-2.4728930	2.9311390	H	128	4.6137240	-4.9964580	-0.7398080
C	90	2.3220520	-5.4090070	-2.2592160					
C	91	1.2957630	-5.7482540	0.0217780					
C	92	3.8162800	-5.5437130	-0.2313870					
H	93	2.3735230	6.4912260	2.4285390	2c_B3LYP				
H	94	3.1280780	4.9282850	2.8136350					
H	95	1.3635100	5.0454470	2.6445730					
H	96	1.3588340	6.8396840	0.0613610	128				
H	97	0.3260430	5.4358920	0.3797270	C	1	0.360947	-8.898453	4.162720
H	98	1.3421140	5.4811840	-1.0820450	C	2	-0.330811	-9.350525	-3.033478
H	99	3.8970330	5.3619250	-0.8440380	C	3	1.811447	-8.878967	-4.164383
H	100	4.6115960	4.9994230	0.7376750	C	4	0.402695	-9.801163	-1.866241
H	101	3.9456960	6.6183000	0.4121070	C	5	-0.107483	-7.724060	-4.877075
H	102	7.9359180	0.4566860	-3.5838430	C	6	-1.515244	-8.644028	-2.577545
H	103	6.2823440	-0.1946710	-3.5898960	C	7	2.517197	-9.312134	-3.036911
H	104	7.4255120	-0.6951260	-2.3292590	C	8	1.798950	-9.782455	-1.868042
H	105	8.6314920	2.0823630	-1.7341810	C	9	-1.247772	-7.048080	-4.441956
H	106	8.0851120	0.9491820	-0.4878800	C	10	-1.966431	-7.517670	-3.266953
H	107	7.4508590	2.6080590	-0.5118460	C	11	2.247192	-7.693115	-4.880264
H	108	6.9102040	2.8445300	-3.5800020	C	12	-0.327820	-9.375854	-0.681168
H	109	5.7532320	3.2947780	-2.3102490	C	13	1.059600	-6.975616	-5.315430

C	14	-1.509811	-8.654541	-1.123245	C	53	0.261459	-2.575455	-1.850006
C	15	3.684158	-8.575348	-2.584549	C	54	-0.520828	-3.118332	-0.533295
C	16	2.521027	-9.338593	-0.685104	C	55	3.630081	-3.974716	-1.091600
C	17	-1.267868	-5.595795	-4.421219	C	56	2.197052	-4.913208	1.197525
C	18	-2.425049	-6.352356	-2.532898	C	57	1.746368	-2.562256	-1.857941
C	19	3.370712	-6.987549	-4.448135	C	58	0.330582	-3.717500	0.516022
C	20	0.364502	-8.953400	0.452667	C	59	2.549591	-3.091492	-0.538391
C	21	1.041519	-5.581543	-5.284775	C	60	1.717743	-3.702881	0.513611
C	22	-1.942291	-7.530960	-0.417160	C	61	-0.493820	-1.640533	-0.923935
C	23	4.104950	-7.438309	-3.275635	C	62	0.342651	-0.739731	-0.047791
C	24	1.820786	-8.934982	0.450912	C	63	-1.695236	-0.880554	-1.482925
C	25	-0.141678	-4.876785	-4.826523	C	64	-0.491379	0.049957	0.922516
C	26	-2.397995	-6.355026	-1.136734	C	65	2.499710	-1.626633	-0.952652
C	27	3.682968	-8.586990	-1.129990	C	66	3.779968	-0.980209	-1.488541
C	28	-1.988968	-5.171143	-3.242447	C	67	1.686432	-0.728638	-0.062729
C	29	3.354416	-5.535187	-4.427612	C	68	2.564850	0.056656	0.895294
C	30	-0.093979	-7.792816	1.197311	O	69	-1.545792	0.244995	-1.915359
C	31	2.207825	-4.846909	-4.830719	O	70	-2.829941	-1.574081	-1.446854
C	32	-1.223618	-7.088852	0.765259	O	71	0.132172	1.138184	1.380829
C	33	4.088303	-7.453430	-0.425278	O	72	3.457153	-0.122635	-2.455109
C	34	-1.549850	-4.046829	-2.524414	O	73	-1.624466	-0.297333	1.205338
C	35	4.536072	-6.260773	-2.543259	O	74	2.755157	-0.676529	1.998703
C	36	2.250946	-7.762543	1.194153	O	75	4.888458	-1.235077	-1.068619
C	37	0.280792	-3.701950	-4.093582	C	76	4.471603	0.719955	-3.139572
C	38	-1.965988	-5.180756	-0.411880	O	77	3.094284	1.109848	0.615509
C	39	4.068695	-5.091171	-3.251358	C	78	3.817719	-0.365707	2.992081
C	40	1.069641	-7.061417	1.652206	C	79	3.608551	1.563202	-4.079773
C	41	1.756363	-3.683700	-4.097916	C	80	5.426971	-0.182892	-3.924286
C	42	-1.231140	-5.639557	0.778717	C	81	5.193420	1.601517	-2.117310
C	43	4.512848	-6.265976	-1.146362	C	82	3.704941	-1.543732	3.961197
C	44	3.361221	-7.030365	0.758865	C	83	3.508224	0.958084	3.692276
C	45	-0.422623	-3.275818	-2.984573	C	84	5.182831	-0.350403	2.298721
C	46	-1.572937	-4.041290	-1.084015	C	85	-4.111343	-1.005966	-1.933792
C	47	3.605103	-3.974884	-2.532532	C	86	-5.098907	-2.142548	-1.662277
C	48	1.051117	-5.662857	1.652313	C	87	-4.009247	-0.712128	-3.432983
C	49	2.448837	-3.242874	-2.989914	C	88	-4.466354	0.235138	-1.110336
C	50	-0.114685	-4.941254	1.202240	C	89	-0.564026	2.131210	2.237839
C	51	4.052261	-5.105300	-0.421021	C	90	0.490875	3.225922	2.405075
C	52	3.331253	-5.581558	0.771393	C	91	-0.923294	1.491226	3.581161

C	92	-1.791000	2.677826	1.500534	3c_B3LYP					
H	93	4.244904	2.228714	-4.672333						
H	94	2.899933	2.172791	-3.510651						
H	95	3.041962	0.923462	-4.763931						
H	96	6.105789	0.436951	-4.520554	128					
H	97	4.867889	-0.830322	-4.608276	C	1	5.6048350	-0.3664460	1.6014090	
H	98	6.023361	-0.805603	-3.254684	C	2	5.8069460	0.8803060	1.0056040	
H	99	5.859177	1.014420	-1.482422	C	3	5.6186760	-1.5734610	0.7867860	
H	100	4.467987	2.114900	-1.479828	C	4	6.0279160	0.9734130	-0.4294520	
H	101	5.788925	2.352463	-2.648911	C	5	4.5866570	-0.5260360	2.6223590	
H	102	4.442352	-1.439163	4.763947	C	6	4.9999670	2.0176050	1.4095490	
H	103	3.886780	-2.489900	3.442200	C	7	5.8259650	-1.4809790	-0.5915800	
H	104	2.706665	-1.582809	4.408920	C	8	6.0324520	-0.1832080	-1.2106470	
H	105	4.242584	1.128708	4.487808	C	9	3.7990130	0.5642530	2.9978680	
H	106	2.514038	0.928467	4.150696	C	10	4.0089940	1.8563390	2.3816560	
H	107	3.554749	1.792450	2.990112	C	11	4.6163270	-2.4821950	1.3107750	
H	108	5.969894	-0.304169	3.059906	C	12	5.3652540	2.1735610	-0.9103370	
H	109	5.286377	0.511795	1.637756	C	13	3.9782300	-1.8360560	2.4460920	
H	110	5.326279	-1.257965	1.705292	C	14	4.7357160	2.8213590	0.2266120	
H	111	-6.105789	-1.841354	-1.969971	C	15	5.0352610	-2.2914120	-1.5013090	
H	112	-5.119888	-2.389252	-0.596298	C	16	5.3674480	-0.1909150	-2.5029410	
H	113	-4.820816	-3.042053	-2.220444	C	17	2.3681900	0.3980550	3.1944280	
H	114	-4.990753	-0.402039	-3.808853	C	18	2.7056290	2.4740920	2.2042070	
H	115	-3.704758	-1.611557	-3.978836	C	19	3.8574300	-3.2668400	0.4380360	
H	116	-3.290970	0.084763	-3.632660	C	20	4.7231860	2.1677800	-2.1522580	
H	117	-5.485962	0.552414	-1.356705	C	21	2.6119370	-1.9981940	2.6615400	
H	118	-3.782532	1.059372	-1.319031	C	22	3.4963720	3.4395110	0.0742720	
H	119	-4.423767	0.003708	-0.041489	C	23	4.0720810	-3.1669050	-0.9980380	
H	120	0.079880	4.046829	3.002151	C	24	4.7246620	0.9590120	-2.9639680	
H	121	0.794739	3.619095	1.430313	C	25	1.7936200	-0.8593240	3.0466640	
H	122	1.380096	2.840546	2.910110	C	26	2.4712800	3.2571750	1.0863630	
H	123	-1.324905	2.257584	4.253632	C	27	4.7453880	-1.4913930	-2.6806400	
H	124	-0.032227	1.060898	4.050507	C	28	1.6784150	1.5543140	2.6738630	
H	125	-1.671417	0.706161	3.458344	C	29	2.4356910	-3.4401790	0.6704710	
H	126	-2.201965	3.520493	2.067688	C	30	3.4341100	2.8137080	-2.3088410	
H	127	-2.566315	1.919083	1.391022	C	31	1.8230420	-2.8241400	1.7696480	
H	128	-1.507019	3.039902	0.506973	C	32	2.8338000	3.4495810	-1.2181800	
					C	33	3.4966780	-1.5881100	-3.3011310	
					C	34	0.4087900	1.4456010	2.0477700	

C	35	2.7787020	-3.2682490	-1.6496810	C	74	-6.0855290	1.1353790	-3.9124010
C	36	3.4306970	0.8545210	-3.6121460	C	75	-4.7045100	3.2252890	-3.6489580
C	37	0.4975520	-0.9777800	2.4454730	C	76	-6.6078130	2.7178820	-2.0256090
C	38	1.1901570	3.1744760	0.4340590	C	77	-3.4336980	-0.5078720	-0.1389400
C	39	1.7744100	-3.4307930	-0.6155290	C	78	-4.5167220	-1.3157050	-0.8108140
C	40	2.6317770	1.9937110	-3.2036050	C	79	-2.3794400	-1.1663810	0.7042610
C	41	0.5200140	-2.2107830	1.6353760	C	80	-2.7974890	-2.3374480	1.5711210
C	42	1.4102210	3.3042710	-0.9881330	O	81	-3.9429230	-2.2031110	-1.6286190
C	43	2.4910770	-2.4880150	-2.7676360	O	82	-2.3821460	-2.1722100	2.8255650
C	44	2.8212100	-0.3899330	-3.7686040	O	83	-5.6990830	-1.1527990	-0.6053450
C	45	-0.2513090	0.1263050	2.0410290	C	84	-4.7110360	-3.2582070	-2.3351500
C	46	0.1518100	2.3662690	0.9119830	O	85	-3.4595330	-3.2611880	1.1426640
C	47	0.5428800	-2.7852600	-0.7429780	C	86	-2.7361350	-3.1283710	3.9063040
C	48	1.2705290	1.8261300	-2.9525090	C	87	-3.6025000	-4.0568140	-3.0231820
C	49	-0.0916830	-2.2096360	0.3990420	C	88	-5.6452290	-2.6117150	-3.3590340
C	50	0.6522120	2.5023430	-1.8425320	C	89	-5.4700710	-4.1274370	-1.3287640
C	51	1.1968140	-1.8314000	-2.8959230	C	90	-2.0596420	-2.5024260	5.1270100
C	52	1.3979700	-0.5468840	-3.5078940	C	91	-2.1503740	-4.5081540	3.5952480
C	53	-1.3675180	-0.0844090	1.0615740	C	92	-4.2575470	-3.1560910	4.0771310
C	54	-0.8576830	1.9332760	-0.0312360	H	93	-2.7968370	6.2966850	3.0895190
C	55	0.2369700	-1.9521010	-1.8906190	H	94	-2.7272450	5.7476620	1.3985560
C	56	0.6225420	0.5375450	-3.0895480	H	95	-1.3284490	5.5124510	2.4662740
C	57	-1.0308750	-1.1516150	-0.0416120	H	96	-2.8603090	4.5199630	4.9723130
C	58	-0.4484820	1.7299570	-1.3449600	H	97	-1.4108320	3.7547390	4.2949930
C	59	-0.6233210	-0.8486480	-1.4805010	H	98	-2.8873820	2.7945320	4.5480140
C	60	-0.4230520	0.4099270	-2.0662970	H	99	-4.9131630	3.1587460	3.0299770
C	61	-2.0065230	1.2210750	0.5874780	H	100	-4.7913820	4.2941150	1.6673180
C	62	-2.6442370	1.9404040	1.8255610	H	101	-4.9432470	4.9097290	3.3283470
C	63	-3.1683240	0.7997670	-0.2970110	H	102	-6.7800910	1.6418960	-4.5907520
C	64	-3.9103600	1.8269960	-1.0758490	H	103	-6.6253500	0.3430540	-3.3870380
O	65	-2.3702390	3.2395390	1.8523100	H	104	-5.2903930	0.6782320	-4.5100950
O	66	-4.5921370	1.3048070	-2.1013280	H	105	-5.3636310	3.7494460	-4.3501500
O	67	-3.3290540	1.3218980	2.6123820	H	106	-3.8885600	2.7741880	-4.2240570
C	68	-2.9812400	4.1542760	2.8487770	H	107	-4.2855970	3.9516740	-2.9514750
O	69	-3.8633790	3.0061670	-0.7705610	H	108	-7.3643450	3.2043950	-2.6514810
C	70	-5.5051490	2.1420470	-2.9192450	H	109	-6.2107940	3.4539020	-1.3246560
C	71	-2.4222550	5.5128420	2.4228230	H	110	-7.0930100	1.9143570	-1.4618360
C	72	-2.5051710	3.7733130	4.2530700	H	111	-4.0364750	-4.8831270	-3.5960850
C	73	-4.5052810	4.1188720	2.7089340	H	112	-2.9127450	-4.4711330	-2.2814780

H	113	-3.0327750	-3.4201460	-3.7078460
H	114	-6.1187940	-3.3928640	-3.9645430
H	115	-5.0861770	-1.9510000	-4.0293890
H	116	-6.4271290	-2.0344020	-2.8622900
H	117	-6.2621690	-3.5621030	-0.8342820
H	118	-4.7891500	-4.5133550	-0.5670380
H	119	-5.9235170	-4.9721200	-1.8601680
H	120	-2.2572010	-3.1113610	6.0154250
H	121	-2.4429390	-1.4925520	5.3022030
H	122	-0.9767490	-2.4396940	4.9818640
H	123	-2.3098270	-5.1690460	4.4546080
H	124	-1.0724080	-4.4358850	3.4167670
H	125	-2.6250340	-4.9545220	2.7198900
H	126	-4.5111050	-3.7520110	4.9609940
H	127	-4.7499210	-3.5954390	3.2080040
H	128	-4.6411250	-2.1415310	4.2270200

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C	1	5.8869130	0.6363560	1.1675950
C	2	5.9527820	1.2749660	-0.0721430
C	3	5.8527660	-0.8176800	1.2354800
C	4	5.9954620	0.4887080	-1.2952650
C	5	5.0148000	1.1549350	2.2063670
C	6	5.1444930	2.4550700	-0.3263700
C	7	5.8858980	-1.5712100	0.0608680
C	8	5.9631660	-0.9053990	-1.2300920
C	9	4.2264470	2.2820520	1.9562390
C	10	4.2908930	2.9394820	0.6674960
C	11	4.9600410	-1.1964390	2.3161520
C	12	5.2220570	1.1873330	-2.3074130
C	13	4.4528900	0.0225810	2.9235650
C	14	4.6953500	2.4018280	-1.7083900
C	15	5.0240540	-2.7313130	-0.0836150
C	16	5.1567060	-1.6588700	-2.1743680

C	17	2.8441810	2.3194020	2.4042210
C	18	2.9470340	3.3714850	0.3253990
C	19	4.1201400	-2.3047880	2.1702970
C	20	4.4442710	0.4643800	-3.2151280
C	21	3.1363770	0.0739390	3.3700950
C	22	3.4114430	2.8373480	-2.0366850
C	23	4.1520130	-3.0824360	0.9492740
C	24	4.4113100	-0.9885620	-3.1475340
C	25	2.3239200	1.2477010	3.1160500
C	26	2.5260450	3.3233950	-0.9944670
C	27	4.5758820	-2.7869060	-1.4659640
C	28	2.0360400	2.9648730	1.3811800
C	29	2.7384960	-2.2369660	2.6158720
C	30	3.1124960	0.9280300	-3.5617120
C	31	2.2708520	-1.0800090	3.2235810
C	32	2.6024450	2.0911300	-2.9826490
C	33	3.2737120	-3.1925310	-1.7552920
C	34	0.7195760	2.5434740	1.1061830
C	35	2.7886260	-3.4837660	0.6464400
C	36	3.0586080	-1.4209420	-3.4514500
C	37	0.9689230	0.8272760	2.8634980
C	38	1.1830820	2.8884400	-1.2916300
C	39	1.8990110	-2.9390200	1.6568290
C	40	2.2579810	-0.2362430	-3.6993310
C	41	0.9369520	-0.6220580	2.9307980
C	42	1.2245300	2.1355870	-2.5216770
C	43	2.3690690	-3.5404120	-0.6739980
C	44	2.4980900	-2.5012820	-2.7683810
C	45	0.1388700	1.4990500	1.9595110
C	46	0.2665580	2.5419100	-0.2975470
C	47	0.5992230	-2.4880200	1.3428230
C	48	0.9480340	-0.1837460	-3.2263880
C	49	0.0775240	-1.3335630	2.0894110
C	50	0.4106030	1.0115750	-2.6339030
C	51	1.0477560	-3.0760750	-1.0136840
C	52	1.1209600	-2.4393780	-2.3067270
C	53	-1.0188820	0.7743110	1.4861360
C	54	-0.8306800	1.6343660	-0.6273450
C	55	0.1477560	-2.5998550	-0.0585240

C	56	0.3610120	-1.2930110	-2.5251630	H	95	-3.0346520	-2.1310650	5.0410650
C	57	-1.0456750	-0.6022660	1.5510300	H	96	-2.7886420	-5.1805060	4.4813350
C	58	-0.6066080	0.6893530	-1.6455850	H	97	-1.5267460	-3.9739260	4.1677830
C	59	-0.8951170	-1.6679480	-0.4759030	H	98	-2.0837540	-5.0424240	2.8576070
C	60	-0.6348160	-0.8308150	-1.5721600	H	99	-4.4074900	-4.7300340	1.8696270
C	61	-1.8865260	1.4930680	0.4666000	H	100	-5.3905130	-3.3355270	2.3527110
C	62	-3.0976520	0.7061680	-0.0104960	H	101	-5.2235180	-4.7288440	3.4484160
C	63	-2.4420020	2.8026480	1.1118560	H	102	-4.2907370	-3.3289320	-4.7346120
C	64	-4.1488790	1.5357590	-0.6880130	H	103	-2.8138590	-2.7863440	-3.9072510
C	65	-1.9291610	-1.3847680	0.6107380	H	104	-4.0215000	-1.5979020	-4.4355390
C	66	-2.4425320	-2.6991220	1.2748560	H	105	-6.5544500	-3.1408660	-3.4994320
C	67	-3.1185210	-0.6280760	0.0461790	H	106	-6.2416520	-1.4187500	-3.2236070
C	68	-4.1974220	-1.5066180	-0.5615590	H	107	-6.5982820	-2.4905300	-1.8462850
O	69	-3.3180920	2.7160590	1.9482780	H	108	-4.7070340	-4.8867430	-2.7478930
O	70	-1.8602810	3.9184330	0.6884290	H	109	-4.8880840	-4.2255730	-1.1092730
O	71	-5.3540430	0.9613030	-0.6654640	H	110	-3.2896040	-4.2677110	-1.8705870
O	72	-2.9040030	-2.4210300	2.4915280	H	111	-1.5066080	7.2270010	0.7058740
O	73	-3.8825600	2.6218410	-1.1723960	H	112	-1.5023780	6.0861270	-0.6571540
O	74	-3.9293670	-1.6926560	-1.8594930	H	113	-0.2700830	5.9544840	0.6145740
O	75	-2.4281550	-3.7792430	0.7251290	H	114	-2.1166370	6.3508480	3.0621970
C	76	-3.4860320	-3.4598030	3.3813910	H	115	-0.8969310	5.0729790	2.9032870
O	77	-5.0869640	-2.0194820	0.0814040	H	116	-2.5858100	4.6503370	3.2735930
C	78	-4.6034340	-2.7364490	-2.6769710	H	117	-3.9434070	6.5774390	1.1273360
C	79	-3.9000620	-2.6392690	4.6040960	H	118	-4.3738550	4.8842120	1.4564090
C	80	-2.3989840	-4.4771470	3.7369620	H	119	-3.8973890	5.3775810	-0.1834930
C	81	-4.7024650	-4.1045390	2.7135470	H	120	-8.6454170	1.0822430	-1.1536560
C	82	-3.8865140	-2.6025270	-4.0218170	H	121	-7.7158940	0.4569970	0.2277200
C	83	-6.0939300	-2.4224140	-2.8117860	H	122	-7.5233560	-0.2778270	-1.3726100
C	84	-4.3562290	-4.1132010	-2.0554150	H	123	-7.3867980	2.3186400	-3.0456950
C	85	-2.2419970	5.2557660	1.2085020	H	124	-6.2435450	0.9717500	-3.1952720
C	86	-1.3212170	6.1869940	0.4174400	H	125	-5.6413690	2.6165760	-2.8897620
C	87	-1.9439580	5.3282560	2.7084230	H	126	-7.7459380	3.3822290	-0.6185190
C	88	-3.7113310	5.5344690	0.8833120	H	127	-5.9988030	3.6994410	-0.6061040
C	89	-6.5642460	1.6638060	-1.1613930	H	128	-6.7422610	2.7567540	0.7048910
C	90	-7.6802040	0.6665880	-0.8455470					
C	91	-6.4429150	1.9102440	-2.6674290					
C	92	-6.7654170	2.9605500	-0.3706190					
H	93	-4.3381840	-3.2958750	5.3630430					
H	94	-4.6413650	-1.8833430	4.3273520					

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C	1	5.9519330	-1.0486350	-1.1519200
C	2	5.8653940	-1.6146160	0.1215680
C	3	6.0001930	0.3956350	-1.3039760
C	4	5.8287580	-0.7596180	1.2969790
C	5	5.1574090	-1.5888430	-2.2418280
C	6	4.9818420	-2.7418780	0.3583240
C	7	5.9606680	1.2181310	-0.1761170
C	8	5.8757010	0.6293560	1.1512680
C	9	4.3068570	-2.6732940	-2.0143540
C	10	4.2167290	-3.2623080	-0.6861580
C	11	5.2350530	0.7483640	-2.4880020
C	12	4.9252510	-1.3580820	2.2611230
C	13	4.7147170	-0.4782360	-3.0675140
C	14	4.3942870	-2.5809170	1.6781220
C	15	5.1535440	2.4248300	-0.1847440
C	16	5.0190920	1.4720230	1.9639590
C	17	2.9792270	-2.6871990	-2.5976520
C	18	2.8342870	-3.6398070	-0.4553080
C	19	4.4578410	1.9091060	-2.4961630
C	20	4.1059660	-0.5478890	3.0487560
C	21	3.4366170	-0.4952960	-3.6315880
C	22	3.0635700	-2.9384940	1.8972320
C	23	4.4159880	2.7649560	-1.3197620
C	24	4.1540210	0.8979320	2.8965370
C	25	2.5523970	-1.6218550	-3.3895160
C	26	2.2624990	-3.4768150	0.8113950
C	27	4.5657210	2.5793980	1.1361470
C	28	2.0724410	-3.2807720	-1.6277040
C	29	3.1293470	1.8884180	-3.0786460
C	30	2.7228810	-0.9254930	3.2803680
C	31	2.6283700	0.7120930	-3.6340620
C	32	2.2081430	-2.0947470	2.7126650
C	33	3.2620200	3.0585720	1.2662820
C	34	0.7788360	-2.7717330	-1.4774360

C	35	3.0622900	3.2708630	-1.1822540
C	36	2.8005800	1.4053270	3.0356640
C	37	1.2025030	-1.1044060	-3.2425460
C	38	0.9107120	-2.9780280	0.9497830
C	39	2.2691270	2.7269420	-2.2581090
C	40	1.9279440	0.2797100	3.2673480
C	41	1.2483380	0.3259050	-3.3918850
C	42	0.8778910	-2.1109710	2.1383980
C	43	2.4901630	3.4085710	0.0868090
C	44	2.3587650	2.4604300	2.2325780
C	45	0.3338180	-1.6617340	-2.2994520
C	46	0.1699450	-2.6553520	-0.1768110
C	47	0.9458320	2.3447150	-2.0119850
C	48	0.6546960	0.2614180	2.6809050
C	49	0.4232010	1.1216740	-2.5901690
C	50	0.1074850	-0.9587540	2.1492980
C	51	1.1113280	3.0384580	0.3163200
C	52	1.0279630	2.4458930	1.6594330
C	53	-0.5581530	-0.8366020	-1.5221110
C	54	-0.8096800	-1.5302520	-0.2141960
C	55	0.3374880	2.5414190	-0.7210770
C	56	0.1784840	1.3785040	1.9051800
C	57	-0.5161030	0.5375950	-1.6644320
C	58	-0.8617110	-0.6150280	1.0776990
C	59	-0.7246570	1.5056640	-0.5289920
C	60	-0.8208320	0.8825310	0.9182890
C	61	-2.0645100	-1.3922110	0.6376000
C	62	-3.1887610	-0.6037340	0.0206900
C	63	-2.5016590	-2.5877980	1.4840370
C	64	-4.2640940	-1.5171160	-0.5391850
C	65	-2.0019790	1.6017730	0.3110070
C	66	-2.4970190	2.8752110	0.9848380
C	67	-3.1555460	0.7329740	-0.1299410
C	68	-4.2018160	1.5189470	-0.8707160
O	69	-2.3970230	-3.7406120	1.1238830
O	70	-2.9977890	-2.1401230	2.6362430
O	71	-3.9462810	-1.8305300	-1.8014400
O	72	-1.7655460	3.9475850	0.6973290
O	73	-5.1706590	-1.9741770	0.1219410

O	74	-5.3970240	0.9235120	-0.8728080	H	113	-3.2251910	-1.4718980	5.1075730
O	75	-3.4609720	2.8297030	1.7230990	H	114	-2.8739340	-4.5564210	5.0333780
C	76	-2.0955370	5.2859150	1.2497920	H	115	-1.6335210	-3.3760070	4.5702950
O	77	-3.9381180	2.5964330	-1.3746090	H	116	-2.1172910	-4.6529600	3.4295640
C	78	-6.6015160	1.5992450	-1.4178190	H	117	-5.2908150	-4.3428250	3.8553990
C	79	-1.0425540	6.1836720	0.5972150	H	118	-4.4102200	-4.5687040	2.3294380
C	80	-1.9354150	5.2631210	2.7721810	H	119	-5.4402270	-3.1411380	2.5509560
C	81	-3.5044610	5.6929980	0.8082010	H	120	-4.1858290	-3.7748730	-4.4919740
C	82	-7.7161610	0.6018410	-1.0982980	H	121	-2.7428730	-3.1617460	-3.6544810
C	83	-6.4445720	1.7963360	-2.9277620	H	122	-3.9030370	-2.0244830	-4.3692390
C	84	-6.8323020	2.9188300	-0.6739630	H	123	-6.5075660	-3.4335550	-3.3944890
C	85	-3.5775460	-3.0511940	3.6567390	H	124	-6.1774960	-1.6943350	-3.3083230
C	86	-4.0590580	-2.0704770	4.7272540	H	125	-6.6176850	-2.5926060	-1.8333580
C	87	-2.4773240	-3.9672910	4.1989270	H	126	-4.7043080	-5.1016940	-2.3697520
C	88	-4.7514530	-3.8264460	3.0532840	H	127	-4.9842590	-4.2642710	-0.8286990
C	89	-4.5903300	-2.9560990	-2.5301170	H	128	-3.3407830	-4.3917050	-1.4783220
C	90	-3.8054160	-2.9793290	-3.8427540					
C	91	-6.0674270	-2.6442250	-2.7745210					
C	92	-4.3929830	-4.2563100	-1.7458540					
H	93	-1.1820650	7.2183830	0.9275450					
H	94	-1.1303700	6.1521590	-0.4932650					
H	95	-0.0322170	5.8650600	0.8706730					
H	96	-2.0665550	6.2769620	3.1666720					
H	97	-0.9326980	4.9176340	3.0453840					
H	98	-2.6749790	4.6092400	3.2376590					
H	99	-4.2673490	5.0852640	1.2965600					
H	100	-3.6071890	5.5828750	-0.2761460					
H	101	-3.6724120	6.7447200	1.0662950					
H	102	-8.6789050	1.0044620	-1.4304830					
H	103	-7.7671600	0.4140670	-0.0216630					
H	104	-7.5454590	-0.3522140	-1.6036820					
H	105	-7.3820840	2.1820810	-3.3438230					
H	106	-6.2235610	0.8418050	-3.4173280					
H	107	-5.6441160	2.5028230	-3.1538030					
H	108	-7.8063960	3.3273190	-0.9654120					
H	109	-6.0610190	3.6533550	-0.9080920					
H	110	-6.8414760	2.7486360	0.4075660					
H	111	-4.5019850	-2.6207440	5.5639810					
H	112	-4.8131140	-1.3914380	4.3175090					

UAM1 level (singlet) optimized cartesian coordinates in angstrom
unit for the systems depicted in Figure 5.

m-1a

6	2.864390	2.466534	-1.426028
6	3.734913	-0.001155	-1.488803
6	3.116464	1.173390	-0.915903
6	1.670338	3.133643	-1.095982
6	2.863692	-2.468576	-1.425139
6	3.116099	-1.175138	-0.915278
6	0.727082	2.554718	-0.220535
6	2.275101	0.732070	0.174234
6	-1.668580	3.134862	-1.095904
6	1.669395	-3.134959	-1.094930
6	2.275438	-0.733532	0.175042
6	-2.862902	2.468645	-1.426361
6	1.147044	1.403749	0.553534
6	-0.725737	2.555052	-0.220279
6	0.726159	-2.555084	-0.219810
6	-3.734025	0.001200	-1.490552
6	1.146603	-1.404987	0.555360
6	-3.115565	1.175181	-0.916631
6	-1.669463	-3.133605	-1.096924
6	-2.863316	-2.466450	-1.427616
6	0.000189	0.785796	1.344509
6	-1.146617	1.405021	0.554742
6	-0.726649	-2.554588	-0.221085
6	-3.115641	-1.173338	-0.917555
6	-0.000638	-0.785835	1.344527
6	-2.275357	0.733533	0.174041
6	-1.147075	-1.403753	0.552902
6	-2.274948	-0.732085	0.173128
6	0.004414	1.407629	2.707252
6	0.001152	0.718878	3.864476
6	-0.005405	-0.718971	3.864455
6	-0.006163	-1.407798	2.707362

1	3.549910	2.914677	-2.158354
1	4.469714	-0.001469	-2.289775
1	1.432995	4.085058	-1.593453
1	3.549937	-2.917739	-2.156146
1	-1.430277	4.086153	-1.593163
1	1.431127	-4.086037	-1.592600
1	-3.548635	2.917615	-2.157965
1	-4.468591	0.001529	-2.291742
1	-1.431940	-4.085099	-1.594154
1	-3.548704	-2.914793	-2.159948
1	0.010184	2.509533	2.697278
1	0.003585	1.236256	4.835758
1	-0.009599	-1.236217	4.835879
1	-0.011282	-2.509658	2.697392

TS1

6	2.516057	2.991834	-1.044129
6	3.923100	0.785800	-0.874186
6	2.978388	1.794455	-0.450309
6	1.173086	3.385907	-0.903783
6	3.633224	-1.810640	-0.833659
6	3.505798	-0.491903	-0.341205
6	0.256691	2.623862	-0.142774
6	2.107612	1.182418	0.525499
6	-2.077845	2.747813	-1.288683
6	2.574645	-2.721500	-0.673730
6	2.430779	-0.248041	0.595743
6	-3.049067	1.855459	-1.772171
6	0.814194	1.589236	0.704841
6	-1.159450	2.362510	-0.286436
6	1.399819	-2.359536	0.021260
6	-3.267902	-0.737990	-2.003761
6	1.438967	-1.163285	0.842531
6	-3.062073	0.512970	-1.307209
6	-0.633830	-3.366058	-1.283805
6	-1.867046	-2.946212	-1.818793

6	-0.238622	0.707579	1.272074
6	-1.485078	1.163359	0.513401
6	0.001170	-2.638850	-0.257012
6	-2.476143	-1.760210	-1.357223
6	0.067805	-0.794091	1.385039
6	-2.346135	0.230519	-0.096252
6	-0.773459	-1.613420	0.409862
6	-1.941080	-1.182317	-0.144327
6	-1.174848	1.334678	2.250745
6	-1.718796	0.533054	3.287072
6	-1.145194	-0.719621	3.575269
6	-0.196502	-1.300976	2.761390
1	3.182624	3.573750	-1.695790
1	4.749476	0.942510	-1.562714
1	0.812037	4.262146	-1.461376
1	4.510471	-2.095914	-1.430224
1	-1.975090	3.736165	-1.759896
1	2.626658	-3.699607	-1.173205
1	-3.723190	2.165440	-2.581413
1	-3.841310	-0.865180	-2.918242
1	-0.122880	-4.230569	-1.731507
1	-2.304883	-3.499527	-2.661152
1	-1.126490	2.424576	2.426162
1	-2.525341	0.933126	3.915105
1	-1.436775	-1.225413	4.510008
1	0.341646	-2.208715	3.063134

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6	2.370294	3.115079	-0.978022
6	3.896849	0.987944	-0.801820
6	2.891523	1.939955	-0.387782
6	1.008315	3.438543	-0.844511
6	3.756129	-1.620668	-0.771573
6	3.546948	-0.313124	-0.276337
6	0.123180	2.624475	-0.097329
6	2.043866	1.274931	0.573450

6	-2.186690	2.670575	-1.260013
6	2.746709	-2.588462	-0.632781
6	2.447581	-0.134892	0.647030
6	-3.101044	1.739424	-1.777909
6	0.727415	1.607498	0.738514
6	-1.279129	2.321598	-0.237531
6	1.542570	-2.293642	0.044849
6	-3.144225	-0.854606	-2.075093
6	1.506341	-1.107194	0.880804
6	-3.031740	0.387154	-1.340876
6	-0.405773	-3.368504	-1.329301
6	-1.641080	-2.993053	-1.892246
6	-0.266089	0.662451	1.276605
6	-1.595392	1.111378	0.603255
6	0.165980	-2.631279	-0.274305
6	-2.313817	-1.844114	-1.428847
6	0.106400	-0.810084	1.393290
6	-2.352103	0.119646	-0.112679
6	-0.672032	-1.649629	0.384696
6	-1.839474	-1.258094	-0.193150
6	-1.391877	1.225133	2.111770
6	-1.963603	0.330606	3.109489
6	-1.267732	-0.818617	3.484497
6	-0.188671	-1.314134	2.763662
1	3.010667	3.736533	-1.619395
1	4.721141	1.192751	-1.480160
1	0.607833	4.302278	-1.394722
1	4.657181	-1.853771	-1.355083
1	-2.117187	3.667649	-1.719603
1	2.858917	-3.559595	-1.135832
1	-3.781961	2.025546	-2.589627
1	-3.684948	-0.990679	-3.007949
1	0.155136	-4.202017	-1.775884
1	-2.030942	-3.550325	-2.755358
1	-1.303996	2.270793	2.485534
1	-2.890279	0.630756	3.612661
1	-1.581382	-1.350684	4.398028
1	0.421310	-2.144414	3.138171

TS2

6	2.173945	3.254303	-0.851916
6	3.801182	1.187781	-0.803876
6	2.757618	2.071783	-0.336766
6	0.807385	3.511511	-0.657683
6	3.806087	-1.426342	-0.840790
6	3.535603	-0.144633	-0.307950
6	-0.029634	2.626475	0.071662
6	1.968160	1.336175	0.615268
6	-2.249006	2.657484	-1.196160
6	2.853402	-2.450417	-0.706850
6	2.450609	-0.051604	0.644330
6	-3.056349	1.690975	-1.836004
6	0.632173	1.595836	0.843666
6	-1.421983	2.313861	-0.108414
6	1.650954	-2.236305	0.004786
6	-3.009680	-0.875176	-2.188455
6	1.577059	-1.084211	0.885536
6	-2.966598	0.344492	-1.455853
6	-0.249328	-3.339393	-1.401651
6	-1.475061	-2.973938	-1.984847
6	-0.214787	0.586506	1.427087
6	-1.793485	1.083207	0.658434
6	0.282827	-2.601624	-0.319425
6	-2.178694	-1.845969	-1.514402
6	0.172368	-0.868524	1.420525
6	-2.302364	0.051529	-0.147403
6	-0.586257	-1.677860	0.366544
6	-1.759437	-1.262761	-0.245184
6	-1.463820	1.021094	2.119361
6	-2.038159	0.037117	3.044735
6	-1.287882	-1.074280	3.427326
6	-0.141076	-1.472443	2.749813
1	2.769913	3.935539	-1.474677
1	4.596785	1.456678	-1.494009
1	0.353845	4.386316	-1.146369
1	4.705889	-1.595231	-1.447764
1	-2.180774	3.666030	-1.629569

1	3.003481	-3.399771	-1.240372
1	-3.652922	1.983370	-2.711575
1	-3.506041	-1.032034	-3.143351
1	0.338305	-4.157116	-1.842146
1	-1.839868	-3.519652	-2.866323
1	-1.433554	2.032005	2.602423
1	-3.020666	0.248723	3.481357
1	-1.619553	-1.662066	4.299081
1	0.502069	-2.281382	3.1115

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6	1.944216	3.383682	-0.688606
6	3.689941	1.410962	-0.798261
6	2.611731	2.210215	-0.261195
6	0.576227	3.550264	-0.421674
6	3.855816	-1.194541	-0.933537
6	3.525388	0.048384	-0.342965
6	-0.194904	2.590136	0.291341
6	1.904020	1.396672	0.683713
6	-2.298268	2.636604	-1.145085
6	2.967532	-2.275533	-0.815992
6	2.473165	0.038876	0.649209
6	-3.027294	1.681234	-1.864508
6	0.554649	1.562029	0.988317
6	-1.582854	2.268279	0.034266
6	1.776737	-2.154052	-0.060291
6	-2.876123	-0.894233	-2.264475
6	1.681905	-1.061957	0.888620
6	-2.917815	0.317154	-1.492977
6	-0.079296	-3.273910	-1.480832
6	-1.313416	-2.942921	-2.060294
6	-0.095079	0.493204	1.657802
6	-2.048218	1.057667	0.696158
6	0.415978	-2.526665	-0.398031
6	-2.040731	-1.840887	-1.571508
6	0.284159	-0.937497	1.457552

6	-2.366000	0.032731	-0.186769
6	-0.482529	-1.616468	0.302345
6	-1.673534	-1.269938	-0.281273
6	-1.505504	0.768637	2.062379
6	-2.090919	-0.324043	2.874340
6	-1.307977	-1.402945	3.282145
6	-0.075649	-1.688041	2.698148
1	2.474303	4.130973	-1.294775
1	4.442337	1.754140	-1.503654
1	0.056541	4.422514	-0.846525
1	4.745709	-1.285758	-1.570919
1	-2.205875	3.661333	-1.530030
1	3.150057	-3.192308	-1.394
1	-3.579719	1.968452	-2.768579
1	-3.319955	-1.042334	-3.245893
1	0.539317	-4.065466	-1.926862
1	-1.664414	-3.484380	-2.949569
1	-1.558666	1.708329	2.690106
1	-3.126912	-0.207510	3.212110
1	-1.684381	-2.062992	4.080330
1	0.590245	-2.477381	3.056142

TS3

6	2.707704	2.900991	-0.609613
6	3.945736	0.579339	-0.703905
6	3.077741	1.606076	-0.172665
6	1.406906	3.370114	-0.374465
6	3.499423	-1.996849	-0.842286
6	3.464188	-0.708922	-0.256879
6	0.424815	2.605715	0.316688
6	2.187208	0.980285	0.762780
6	-1.538946	3.052870	-1.236951
6	2.392358	-2.851416	-0.719001
6	2.429995	-0.471386	0.724000
6	-2.423671	2.258673	-1.978614
6	0.907453	1.452632	1.053489

6	-0.984567	2.574067	-0.013801
6	1.252373	-2.464343	0.028206
6	-2.885354	-0.292291	-2.304296
6	1.401839	-1.356088	0.948872
6	-2.647924	0.921394	-1.572536
6	-0.786545	-3.236637	-1.353902
6	-1.903711	-2.659696	-1.969888
6	0.015300	0.560813	1.719484
6	-1.720826	1.500842	0.635036
6	-0.154905	-2.587318	-0.273609
6	-2.359927	-1.391632	-1.534338
6	0.086659	-0.885089	1.475418
6	-2.236978	0.557588	-0.233234
6	-0.889199	-1.528581	0.445499
6	-1.942448	-0.893873	-0.244481
6	-1.325203	1.139433	2.037638
6	-2.225984	0.206985	2.763305
6	-1.948379	-1.119390	2.910130
6	-0.836150	-1.746716	2.261233
1	3.407565	3.507056	-1.200813
1	4.764111	0.740612	-1.400817
1	1.103236	4.333866	-0.810599
1	4.345556	-2.291020	-1.478225
1	-1.200598	4.018011	-1.638220
1	2.370801	-3.793143	-1.285554
1	-2.847429	2.632206	-2.920050
1	-3.303943	-0.364038	-3.305054
1	-0.344743	-4.154187	-1.767810
1	-2.361835	-3.137146	-2.846215
1	-1.212537	2.076117	2.656483
1	-3.124923	0.654659	3.209842
1	-2.612248	-1.765608	3.506104
1	-0.538941	-2.767745	2.531683

TS4

6	-2.490450	-2.938559	-0.974016
6	-3.840449	-0.687282	-0.965875
6	-2.948738	-1.704275	-0.457242
6	-1.172132	-3.341313	-0.723668
6	-3.506538	1.910068	-0.927897
6	-3.439057	0.590848	-0.422652
6	-0.269343	-2.575934	0.068668
6	-2.132433	-1.105879	0.565471
6	1.755807	-2.753921	-1.475311
6	-2.452220	2.812570	-0.697341
6	-2.434776	0.333166	0.585113
6	2.655628	-1.868279	-2.085265
6	-0.858497	-1.544252	0.905557
6	1.140154	-2.425635	-0.232283
6	-1.330655	2.436448	0.076111
6	3.061115	0.712059	-2.134153
6	-1.452290	1.242316	0.879929
6	2.828223	-0.574281	-1.535499
6	0.756583	3.448378	-1.070005
6	1.942440	2.985744	-1.656719
6	-0.015108	-0.663766	1.681016
6	1.815502	-1.405574	0.547897
6	0.091618	2.660913	-0.112626
6	2.434159	1.711131	-1.309415
6	-0.129531	0.823069	1.450689
6	2.334307	-0.355229	-0.194318
6	0.808186	1.552441	0.522583
6	1.931813	1.064595	-0.102235
6	1.352774	-1.244037	1.948523
6	2.086217	-0.371480	2.909466
6	1.321757	0.594991	3.479879
6	-0.013118	0.743298	2.930736
1	-3.130063	-3.536098	-1.637414
1	-4.618958	-0.842476	-1.708363
1	-0.786525	-4.242207	-1.224574
1	-4.334007	2.204347	-1.588272
1	1.461368	-3.676706	-1.993889

1	-2.461284	3.789931	-1.200316
1	3.132141	-2.133743	-3.038151
1	3.543282	0.893257	-3.091591
1	0.297844	4.382494	-1.423476
1	2.425550	3.565485	-2.454956
1	1.255050	-2.260519	2.432917
1	3.128985	-0.588721	3.153727
1	1.640849	1.232505	4.312040
1	-0.878022	0.963099	3.561857

m-3a

6	-2.694220	-2.679030	-1.146548
6	-3.867859	-0.341090	-1.029653
6	-3.063552	-1.446448	-0.562973
6	-1.406901	-3.180079	-0.918109
6	-3.321850	2.215629	-0.873744
6	-3.370773	0.874928	-0.427714
6	-0.463535	-2.521926	-0.077650
6	-2.212869	-0.966419	0.498667
6	1.538015	-2.719213	-1.654046
6	-2.203884	3.023855	-0.591060
6	-2.400235	0.488611	0.572501
6	2.519581	-1.872895	-2.190498
6	-0.992820	-1.530121	0.843423
6	0.949582	-2.439423	-0.387933
6	-1.124058	2.528055	0.171876
6	3.166078	0.652035	-2.037764
6	-1.344500	1.297458	0.894541
6	2.804038	-0.647865	-1.540342
6	1.065230	3.476351	-0.831274
6	2.234231	2.970875	-1.415022
6	-0.092406	-0.773715	1.718948
6	1.699261	-1.539197	0.466169
6	0.316035	2.674573	0.049293
6	2.618701	1.640355	-1.146846
6	-0.074814	0.752979	1.447915

6	2.316289	-0.484472	-0.188744	6	0.574740	-2.616946	-0.095377
6	0.940274	1.483198	0.638887	6	-0.779004	2.557685	0.270662
6	2.042828	0.955493	0.004451	6	2.764881	-0.019072	-2.386843
6	1.254226	-1.499439	1.870594	6	-1.160505	1.422334	1.101187
6	1.993162	-0.754674	2.942770	6	2.419450	-1.175918	-1.615076
6	1.193286	0.151163	3.543002	6	1.118133	3.145745	-1.306022
6	-0.132151	0.244658	2.864730	6	2.078625	2.439607	-2.035035
1	-3.369557	-3.191814	-1.844442	6	-0.184304	-0.688348	1.856455
1	-4.649368	-0.401700	-1.782652	6	1.433225	-1.647382	0.570955
1	-1.074145	-4.070194	-1.473110	6	0.619300	2.607647	-0.088127
1	-4.113262	2.604253	-1.529733	6	2.440714	1.140396	-1.609766
1	1.164923	-3.566039	-2.246425	6	-0.172585	0.685201	1.859494
1	-2.135816	4.022524	-1.045390	6	2.114761	-0.762457	-0.253150
1	2.978229	-2.104979	-3.160717	6	1.458017	1.620110	0.576566
1	3.679182	0.857738	-2.973877	6	2.127134	0.726850	-0.250006
1	0.683015	4.461848	-1.132375	6	1.111222	-1.437137	2.025997
1	2.784217	3.566334	-2.156205	6	2.153500	-0.688927	2.775199
1	1.083187	-2.550664	2.243628	6	2.163603	0.647070	2.778468
1	3.024720	-1.005942	3.192557	6	1.132814	1.413760	2.031843
1	1.427225	0.787677	4.397316	1	-3.831965	-2.920255	-1.404157
1	-1.020105	0.454114	3.480031	1	-4.718026	0.038629	-1.525069
<hr/>				1	-1.685986	-4.090669	-0.987151
m-4a				1	-3.773723	2.981996	-1.414006
6	-3.079906	-2.455823	-0.751750	1	0.608851	-4.073200	-1.723754
6	-3.915455	0.033241	-0.792138	1	-1.612606	4.115492	-0.991504
6	-3.265623	-1.143622	-0.266032	1	2.406911	-2.865902	-2.996955
6	-1.871765	-3.123324	-0.496656	1	3.120001	-0.020060	-3.414680
6	-3.035244	2.504984	-0.754841	1	0.685823	4.071852	-1.708396
6	-3.243961	1.199459	-0.271965	1	2.463220	2.836837	-2.983790
6	-0.821268	-2.542124	0.268586	1	0.935411	-2.432267	2.522712
6	-2.321280	-0.707061	0.741361	1	2.899208	-1.292388	3.311653
6	1.059875	-3.157737	-1.317510	1	2.918114	1.236853	3.317685
6	-1.815066	3.153991	-0.495881	1	0.972853	2.410409	2.530593
6	-2.300616	0.743694	0.735888				
6	2.031810	-2.466028	-2.045521				
6	-1.182246	-1.409201	1.105742				

B3LYP/6-31G(d) optimized cartesian coordinates in angstrom unit

for the systems depicted in Figure 6.

1a

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C	1	0.797806	-4.406433	2.765991
C	2	1.495346	-4.843216	1.637695
C	3	-0.658127	-4.406082	2.766479
C	4	0.766769	-5.291000	0.462845
C	5	1.247940	-3.233032	3.488663
C	6	2.673172	-4.122100	1.188446
C	7	-1.356644	-4.842560	1.638672
C	8	-0.629150	-5.290665	0.463333
C	9	2.381622	-2.538910	3.060410
C	10	3.108643	-2.993561	1.885696
C	11	-1.107178	-3.232498	3.489502
C	12	1.494492	-4.844788	-0.713074
C	13	0.070709	-2.501465	3.929871
C	14	2.672653	-4.123062	-0.265700
C	15	-2.534424	-4.120895	1.190323
C	16	-1.357468	-4.844116	-0.712051
C	17	2.385071	-1.087692	3.054733
C	18	3.556793	-1.819900	1.156540
C	19	-2.240784	-2.537827	3.062088
C	20	0.796158	-4.409454	-1.841476
C	21	0.071106	-1.106888	3.909332
C	22	3.107605	-2.995438	-0.964706
C	23	-2.968842	-2.992111	1.887863
C	24	-0.659744	-4.409119	-1.840958
C	25	1.247238	-0.382309	3.463135
C	26	3.556320	-1.820816	-0.237396
C	27	-2.534973	-4.121796	-0.263840
C	28	3.102356	-0.645828	1.884674
C	29	-2.243500	-1.086563	3.056244
C	30	1.245789	-3.236969	-2.566025

C	31	-1.105042	-0.381714	3.463867
C	32	2.379745	-2.542328	-2.139542
C	33	-2.969864	-2.994019	-0.962524
C	34	2.644379	0.476593	1.184006
C	35	-3.416992	-1.818237	1.159027
C	36	-1.109283	-3.236359	-2.565200
C	37	0.812027	0.794327	2.744400
C	38	3.101212	-0.647720	-0.966782
C	39	-2.961258	-0.644394	1.886703
C	40	0.068268	-2.505981	-3.007431
C	41	-0.669724	0.794739	2.744934
C	42	2.383148	-1.091034	-2.135696
C	43	-3.417480	-1.819168	-0.234940
C	44	-2.242661	-2.541229	-2.137924
C	45	1.502991	1.222549	1.635544
C	46	2.643723	0.475586	-0.267136
C	47	-2.503326	0.477844	1.185684
C	48	0.068604	-1.111420	-2.988739
C	49	-1.361069	1.223236	1.636383
C	50	1.245026	-0.386200	-2.544235
C	51	-2.962463	-0.646271	-0.964600
C	52	-2.245377	-1.089951	-2.134048
C	53	0.878800	2.012573	0.458008
C	54	1.501953	1.220840	-0.718735
C	55	-2.503891	0.476868	-0.265350
C	56	-1.107224	-0.385696	-2.543472
C	57	-0.737808	2.012924	0.458450
C	58	0.810318	0.791412	-1.826767
C	59	-1.362091	1.221542	-0.717804
C	60	-0.671417	0.791672	-1.826187
C	61	1.495148	3.409515	0.456329
C	62	0.800293	4.552048	0.456421
C	63	-0.657852	4.552414	0.457504
C	64	-1.353700	3.410629	0.457626
H	65	2.582062	3.421051	0.456345
H	66	1.324646	5.503937	0.454651
H	67	-1.181534	5.504715	0.457291
H	68	-2.440567	3.423600	0.457047

3a

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C	1	-0.701294	-3.860428	2.723816
C	2	0.318787	-4.559006	2.075943
C	3	-2.012314	-3.741470	2.101730
C	4	0.074051	-5.163651	0.777115
C	5	-0.408585	-2.607544	3.394211
C	6	1.673431	-4.034286	2.079086
C	7	-2.245560	-4.325104	0.852737
C	8	-1.180573	-5.045822	0.176956
C	9	0.886673	-2.090973	3.383835
C	10	1.951462	-2.824097	2.720856
C	11	-2.531677	-2.419464	2.395187
C	12	1.279572	-5.018326	-0.020676
C	13	-1.533203	-1.715530	3.186569
C	14	2.269592	-4.324951	0.784729
C	15	-3.004196	-3.603210	-0.153275
C	16	-1.281509	-4.767960	-1.247375
C	17	1.108215	-0.671234	3.153015
C	18	2.833755	-1.857910	2.092728
C	19	-3.273422	-1.729568	1.432190
C	20	1.184830	-4.755936	-1.389313
C	21	-1.304276	-0.359300	2.961136
C	22	3.129608	-3.400970	0.189407
C	23	-3.500748	-2.332825	0.130875
C	24	-0.123779	-4.623886	-2.014389
C	25	0.034409	0.194153	2.928192
C	26	3.418686	-2.147354	0.861832
C	27	-2.402786	-3.868210	-1.450714
C	28	2.298904	-0.529648	2.361603
C	29	-3.059296	-0.310120	1.231827
C	30	2.078568	-3.795883	-2.008896
C	31	-2.087967	0.352371	1.985260
C	32	3.034866	-3.129745	-1.237595
C	33	-2.313110	-2.849121	-2.402542
C	34	2.339874	0.463058	1.381348
C	35	-3.394348	-1.278366	-0.861800

C	36	-0.039841	-3.574875	-3.012680
C	37	0.087646	1.273987	1.935242
C	38	3.500732	-1.112015	-0.150665
C	39	-3.122681	-0.035600	-0.185532
C	40	1.322739	-3.065384	-3.012238
C	41	-1.316284	1.417709	1.418167
C	42	3.276718	-1.714096	-1.445938
C	43	-2.800980	-1.516098	-2.090637
C	44	-1.112656	-2.699646	-3.196533
C	45	1.253082	1.414000	1.168198
C	46	2.972610	0.153412	0.113007
C	47	-2.321091	0.970734	-0.743454
C	48	1.553574	-1.705750	-3.206558
C	49	-1.669067	1.896591	0.162766
C	50	2.555817	-1.011719	-2.420883
C	51	-1.888519	-0.533798	-2.659546
C	52	-0.872070	-1.276627	-3.369003
C	53	1.378600	1.868027	-0.283539
C	54	2.285812	0.878723	-0.907990
C	55	-1.597565	0.696884	-2.015015
C	56	0.434006	-0.797974	-3.394196
C	57	0.194305	2.304871	-1.221146
C	58	2.069061	0.326218	-2.156296
C	59	-0.243393	1.254898	-2.183456
C	60	0.734634	0.459686	-2.776825
C	61	1.387497	3.223953	-1.002625
C	62	0.898987	4.360168	-0.168503
C	63	-0.376022	4.185806	0.190552
C	64	-0.970413	3.007202	-0.533752
H	65	2.187775	3.359985	-1.724167
H	66	1.554337	5.163651	0.151642
H	67	-0.952133	4.820221	0.855118
H	68	-1.645172	3.386444	-1.317032

TS5

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C	1	0.508118	-4.401337	2.260605
C	2	1.176727	-4.858582	1.123016
C	3	-0.945190	-4.289917	2.256805
C	4	0.424026	-5.221359	-0.065796
C	5	1.040512	-3.282867	3.013306
C	6	2.407227	-4.214874	0.696915
C	7	-1.667480	-4.643494	1.114212
C	8	-0.969223	-5.110458	-0.069702
C	9	2.218719	-2.656800	2.600815
C	10	2.919296	-3.136490	1.421387
C	11	-1.309906	-3.110031	3.014160
C	12	1.189377	-4.801620	-1.225677
C	13	-0.081543	-2.480545	3.469467
C	14	2.416321	-4.182297	-0.756729
C	15	-2.780853	-3.816025	0.679749
C	16	-1.652740	-4.577377	-1.236100
C	17	2.318832	-1.208145	2.620193
C	18	3.456589	-1.981903	0.721237
C	19	-2.385361	-2.313217	2.599533
C	20	0.533768	-4.288971	-2.348694
C	21	0.021667	-1.091766	3.473618
C	22	2.941437	-3.075897	-1.427521
C	23	-3.128159	-2.677246	1.404327
C	24	-0.917221	-4.171692	-2.351837
C	25	1.232086	-0.434753	3.037186
C	26	3.471298	-1.954269	-0.673004
C	27	-2.771454	-3.774400	-0.774155
C	28	3.076935	-0.795197	1.467773
C	29	-2.292038	-0.871078	2.645279
C	30	1.079269	-3.139587	-3.043106
C	31	-1.095932	-0.269623	3.056854
C	32	2.263443	-2.545074	-2.598969
C	33	-3.110153	-2.596985	-1.441849
C	34	2.700668	0.371368	0.789383
C	35	-3.471298	-1.450867	0.705688

C	36	-1.269730	-2.949921	-3.049011
C	37	0.863968	0.798233	2.351654
C	38	3.122177	-0.733475	-1.380325
C	39	-2.953049	-0.334518	1.465805
C	40	-0.034943	-2.309982	-3.473618
C	41	-0.606369	0.928177	2.442719
C	42	2.381622	-1.097534	-2.564987
C	43	-3.464691	-1.407242	-0.684784
C	44	-2.341660	-2.173126	-2.597794
C	45	1.601608	1.177856	1.241226
C	46	2.749786	0.411743	-0.663132
C	47	-2.465271	0.811539	0.839462
C	48	0.078339	-0.922623	-3.428635
C	49	-1.419006	1.621200	1.504471
C	50	1.306961	-0.299408	-2.970352
C	51	-2.902161	-0.251251	-1.357132
C	52	-2.225311	-0.729523	-2.547012
C	53	1.105637	2.064468	0.048660
C	54	1.705292	1.280289	-1.127563
C	55	-2.387085	0.830353	-0.616867
C	56	-1.036270	-0.120926	-2.955948
C	57	-0.413345	2.175217	-0.074066
C	58	0.962570	0.894180	-2.226929
C	59	-1.162506	1.467896	-1.085419
C	60	-0.509689	0.986206	-2.212738
C	61	1.645172	3.469910	0.277786
C	62	0.965408	4.313690	1.149307
C	63	-0.317032	4.034744	1.605377
C	64	-1.133957	3.002258	0.916092
H	65	2.617400	3.729797	-0.127960
H	66	1.459793	5.221359	1.490036
H	67	-0.794952	4.653229	2.358383
H	68	-2.066635	3.432968	0.536652

B3LYP/6-31G(d) optimized cartesian coordinates in angstrom unit

for the systems depicted in Figure 7.

1a (T)

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C	1	-3.0297500	-0.7194310	2.3213470
C	2	-3.4588800	-1.4253500	1.1807500
C	3	-3.0296570	0.7224750	2.3204910
C	4	-3.8952130	-0.6961230	-0.0004880
C	5	-1.8571900	-1.1726360	3.0482580
C	6	-2.7298790	-2.5827770	0.7353070
C	7	-3.4586530	1.4270380	1.1789810
C	8	-3.8951220	0.6964500	-0.0013290
C	9	-1.1612020	-2.3038500	2.6218580
C	10	-1.6044480	-3.0273400	1.4370320
C	11	-1.8570410	1.1764670	3.0467540
C	12	-3.4582570	-1.4268720	-1.1807620
C	13	-1.1265460	0.0020910	3.4966570
C	14	-2.7295470	-2.5837220	-0.7335290
C	15	-2.7294460	2.5838440	0.7322080
C	16	-3.4580250	1.4257430	-1.1824400
C	17	0.2888910	-2.3021060	2.6167940
C	18	-0.4314320	-3.4639780	0.7169600
C	19	-1.1609150	2.3070660	2.6191860
C	20	-3.0285370	-0.7222820	-2.3218710
C	21	0.2679770	0.0021350	3.4842000
C	22	-1.6036950	-3.0292180	-1.4341320
C	23	-1.6040060	3.0291230	1.4333580
C	24	-3.0284610	0.7197270	-2.3227830
C	25	0.9945190	-1.1713550	3.0332160
C	26	-0.4310790	-3.4650200	-0.7127710
C	27	-2.7293140	2.5830620	-0.7366540
C	28	0.7262010	-3.0158770	1.4338800
C	29	0.2891670	2.3051210	2.6140870
C	30	-1.8555470	-1.1763470	-3.0475860

C	31	0.9945440	1.1750550	3.0321540
C	32	-1.1597750	-2.3069430	-2.6194260
C	33	-1.6033140	3.0276120	-1.4377070
C	34	1.8572170	-2.5481200	0.7337410
C	35	-0.4309150	3.4649650	0.7127570
C	36	-1.8554140	1.1727450	-3.0489000
C	37	2.1701060	-0.7261100	2.3101690
C	38	0.7269010	-3.0174980	-1.4293730
C	39	0.7266540	3.0178100	1.4302230
C	40	-1.1246460	-0.0020640	-3.4968810
C	41	2.1702570	0.7286830	2.3089960
C	42	0.2903770	-2.3053890	-2.6139520
C	43	-0.4307650	3.4642460	-0.7170350
C	44	-1.1595110	2.3039340	-2.6221440
C	45	2.5986510	-1.4284800	1.1829510
C	46	1.8574960	-2.5491900	-0.7292680
C	47	1.8576300	2.5489860	0.7305120
C	48	0.2699540	-0.0021580	-3.4836990
C	49	2.5987090	1.4295580	1.1813520
C	50	0.9960490	-1.1752710	-3.0311340
C	51	0.7273210	3.0157000	-1.4331600
C	52	0.2904540	2.3021480	-2.6166750
C	53	3.3771890	-0.8022550	0.0014870
C	54	2.5990540	-1.4298730	-1.1794140
C	55	1.8575410	2.5480360	-0.7324800
C	56	0.9961570	1.1714040	-3.0326050
C	57	3.3770670	0.8018900	0.0002270
C	58	2.1716680	-0.7289140	-2.3078170
C	59	2.5990200	1.4278440	-1.1811260
C	60	2.1715880	0.7257440	-2.3086170
C	61	4.7746860	-1.4247370	0.0017290
C	62	5.9173610	-0.7291080	-0.0000010
C	63	5.9173100	0.7290360	-0.0008390
C	64	4.7747130	1.4246870	-0.0009850
H	65	4.7827010	-2.5112930	0.0010160
H	66	6.8695030	-1.2527990	-0.0020640
H	67	6.8696070	1.2526400	-0.0014340
H	68	4.7806970	2.5112480	0.0022560

TS6

68

C	1	2.7517020	0.5676260	2.6255230
C	2	3.3207930	1.3019830	1.5843830
C	3	2.7213800	-0.8868880	2.5585440
C	4	3.8827920	0.6169270	0.4310200
C	5	1.5128540	1.0116940	3.2363430
C	6	2.6726270	2.5121590	1.1090270
C	7	3.2662470	-1.5434220	1.4515730
C	8	3.8545640	-0.7776770	0.3676250
C	9	0.8882980	2.1755100	2.7790870
C	10	1.4808920	2.9399500	1.6933980
C	11	1.4682740	-1.3349520	3.1281130
C	12	3.5865160	1.4052480	-0.7500960
C	13	0.7182760	-0.1650570	3.5433500
C	14	2.8399130	2.5751790	-0.3354740
C	15	2.5706180	-2.6770340	0.8647480
C	16	3.5329140	-1.4434680	-0.8843660
C	17	-0.5505130	2.2049480	2.6071440
C	18	0.4023030	3.4425090	0.8566510
C	19	0.7928060	-2.4267530	2.5602000
C	20	3.2746380	0.7651540	-1.9579550
C	21	-0.6688020	-0.1303390	3.3765910
C	22	1.8054140	3.0681720	-1.1370860
C	23	1.3604880	-3.1074840	1.4058600
C	24	3.2482330	-0.6829560	-2.0261900
C	25	-1.3133670	1.0738940	2.8984750
C	26	0.5665350	3.5093720	-0.5332900
C	27	2.7443610	-2.6180870	-0.5798060
C	28	-0.8455210	2.9899340	1.4214090
C	29	-0.6383600	-2.3891660	2.3932850
C	30	2.2006260	1.2746470	-2.7881000
C	31	-1.3685820	-1.2618470	2.7879990
C	32	1.4802240	2.4024840	-2.3916150
C	33	1.6980170	-3.0013690	-1.4254780
C	34	-1.8892520	2.5816170	0.5734110
C	35	0.2701670	-3.4987180	0.5264310

C	36	2.1595490	-1.0750690	-2.9013260
C	37	-2.4099770	0.6768030	2.0265090
C	38	-0.5220570	3.1133340	-1.4113270
C	39	-0.9620010	-3.0589980	1.1281860
C	40	1.5055110	0.1367780	-3.3693330
C	41	-2.4577820	-0.7568620	1.9825810
C	42	0.0394930	2.4397790	-2.5564230
C	43	0.4426570	-3.4545510	-0.8664440
C	44	1.4006620	-2.2101440	-2.6119320
C	45	-2.6829260	1.4408240	0.8863160
C	46	-1.7281650	2.6500500	-0.8703220
C	47	-1.9862220	-2.5522420	0.3282410
C	48	0.1190940	0.1688650	-3.5172040
C	49	-2.8105030	-1.4397080	0.7643130
C	50	-0.6343100	1.3399330	-3.1019060
C	51	-0.6238330	-2.9401740	-1.6983330
C	52	-0.0397440	-2.1809050	-2.7794350
C	53	-3.3266650	0.8770500	-0.3970440
C	54	-2.4498420	1.5597780	-1.4671010
C	55	-1.8126310	-2.4853080	-1.1074500
C	56	-0.6722330	-1.0109260	-3.2174350
C	57	-3.2971350	-0.6965860	-0.4787790
C	58	-1.8947180	0.8997690	-2.5453840
C	59	-2.4756870	-1.3099060	-1.5978530
C	60	-1.9163930	-0.5776330	-2.6204680
C	61	-4.7315280	1.4350860	-0.2901860
C	62	-5.7915880	0.6825780	0.1507030
C	63	-5.7112960	-0.7223420	0.2884830
C	64	-4.5681900	-1.4109480	-0.1351320
H	65	-4.8372870	2.5020940	-0.4593180
H	66	-6.7433040	1.1717660	0.3418090
H	67	-6.5859920	-1.2848620	0.6001180
H	68	-4.6311120	-2.4616900	-0.3940920

15

68

C	1	2.6488000	0.2005450	2.7562230
C	2	3.2697290	1.0480750	1.8376970
C	3	2.6006790	-1.2343740	2.5064660
C	4	3.8707790	0.5004630	0.6321670
C	5	1.3932750	0.5897590	3.3696220
C	6	2.6582580	2.3203690	1.4948210
C	7	3.1833650	-1.7592340	1.3500760
C	8	3.8250940	-0.8756950	0.3946760
C	9	0.8042910	1.8130900	3.0418960
C	10	1.4505300	2.6960400	2.0844780
C	11	1.3212850	-1.7285300	2.9688060
C	12	3.6294370	1.4325370	-0.4527570
C	13	0.5704320	-0.6022270	3.4938770
C	14	2.8809160	2.5574710	0.0777470
C	15	2.4981450	-2.8016030	0.6034830
C	16	3.5441240	-1.3748860	-0.9411440
C	17	-0.6284130	1.8901880	2.8226910
C	18	0.4124620	3.3162600	1.2773770
C	19	0.6520330	-2.7281910	2.2456730
C	20	3.3548530	0.9540750	-1.7386180
C	21	-0.8038510	-0.5220640	3.2762640
C	22	1.8853690	3.1615430	-0.6937340
C	23	1.2602950	-3.2719470	1.0402090
C	24	3.3125740	-0.4773880	-1.9873390
C	25	-1.4135190	0.7414800	2.9326240
C	26	0.6269060	3.5462340	-0.0833590
C	27	2.7275150	-2.5673540	-0.8145430
C	28	-0.8666500	2.8139430	1.7363040
C	29	-0.7726960	-2.6579500	2.0392680
C	30	2.3199080	1.5800980	-2.5378250
C	31	-1.5019330	-1.5631620	2.5321240
C	32	1.5995920	2.6636370	-2.0309130
C	33	1.7136690	-2.8235720	-1.7391720
C	34	-1.8804330	2.5322040	0.8083520
C	35	0.2040000	-3.5320080	0.0786960

C	36	2.2545090	-0.7383850	-2.9451940
C	37	-2.4778620	0.4711410	1.9772250
C	38	-0.4336030	3.2831890	-1.0436910
C	39	-1.0538150	-3.1487290	0.6835440
C	40	1.6344220	0.5335000	-3.2794190
C	41	-2.5646940	-0.9624530	1.7811140
C	42	0.1653730	2.7441650	-2.2397700
C	43	0.4275820	-3.3215120	-1.2848980
C	44	1.4703030	-1.8879120	-2.8264920
C	45	-2.6996250	1.3690020	0.9436160
C	46	-1.6663570	2.7794100	-0.6079750
C	47	-2.0474440	-2.5624620	-0.0787870
C	48	0.2545240	0.6067580	-3.4686460
C	49	-2.9869380	-1.5347380	0.4908770
C	50	-0.4989610	1.7298180	-2.9379890
C	51	-0.6014760	-2.6928890	-2.0818980
C	52	0.0364160	-1.8142560	-3.0364310
C	53	-3.3157810	0.9865420	-0.4249140
C	54	-2.3821380	1.7841130	-1.3607400
C	55	-1.8079070	-2.3013100	-1.4754420
C	56	-0.5607540	-0.5870360	-3.3444280
C	57	-3.2601600	-0.5417380	-0.7043640
C	58	-1.7846120	1.2465090	-2.4831940
C	59	-2.4236480	-1.0480830	-1.8307400
C	60	-1.8181540	-0.2104530	-2.7392750
C	61	-4.7548140	1.4687890	-0.3577660
C	62	-5.7478390	0.6403960	0.1492030
C	63	-5.5597400	-0.7208650	0.3626280
C	64	-4.3778900	-1.4059910	-0.1956510
H	65	-4.9411700	2.5227280	-0.5374580
H	66	-6.7154150	1.0762820	0.3895430
H	67	-6.3470630	-1.3248040	0.8034330
H	68	-4.6147900	-2.2882640	-0.7918310

TS7

68

C	1	2.6370920	-0.6121460	2.7045750
C	2	3.2561440	0.4736190	2.0819960
C	3	2.6059360	-1.9110760	2.0444660
C	4	3.8678340	0.3095830	0.7737730
C	5	1.3729910	-0.4297170	3.3918920
C	6	2.6350260	1.7863360	2.1257350
C	7	3.1980690	-2.0679460	0.7886340
C	8	3.8341780	-0.9356600	0.1396770
C	9	0.7697950	0.8292110	3.4272330
C	10	1.4169980	1.9614240	2.7858790
C	11	1.3287900	-2.5329700	2.3316320
C	12	3.6250960	1.5202090	0.0107890
C	13	0.5629670	-1.6115810	3.1527380
C	14	2.8660010	2.4351050	0.8450920
C	15	2.5233670	-2.8488130	-0.2353660
C	16	3.5587320	-1.0185130	-1.2847540
C	17	-0.6620440	0.9569420	3.2176170
C	18	0.3812050	2.7885300	2.1895850
C	19	0.6778470	-3.2885510	1.3467360
C	20	3.3606120	1.4423000	-1.3599560
C	21	-0.8083630	-1.4763580	2.9434580
C	22	1.8728780	3.2370780	0.2786330
C	23	1.2916570	-3.4412470	0.0377930
C	24	3.3237720	0.1457140	-2.0195620
C	25	-1.4375300	-0.1767780	2.9649740
C	26	0.6064120	3.4175000	0.9648630
C	27	2.7460140	-2.1997630	-1.5179090
C	28	-0.8988180	2.1586870	2.4591190
C	29	-0.7513180	-3.1782710	1.1603090
C	30	2.3287700	2.2747510	-1.9464070
C	31	-1.4809650	-2.2686840	1.9345700
C	32	1.6009440	3.1612310	-1.1480210
C	33	1.7296080	-2.1720380	-2.4735070
C	34	-1.8995040	2.1574840	1.4792820

C	35	0.2330770	-3.4027190	-0.9559030
C	36	2.2691030	0.1753030	-3.0152430
C	37	-2.5041300	-0.1680850	1.9685850
C	38	-0.4452500	3.4545650	-0.0377280
C	39	-1.0284150	-3.2349430	-0.2694970
C	40	1.6517690	1.4910510	-2.9675320
C	41	-2.5742060	-1.5193620	1.3847850
C	42	0.1669860	3.2992920	-1.3360780
C	43	0.4427390	-2.7848120	-2.1853140
C	44	1.4825020	-0.9601480	-3.2328420
C	45	-2.7128290	0.9973110	1.2455380
C	46	-1.6803860	2.8422210	0.2163750
C	47	-2.0654570	-2.4868260	-0.8205050
C	48	0.2748730	1.6175320	-3.1366780
C	49	-3.0433610	-1.8176580	0.0711980
C	50	-0.4861200	2.5386210	-2.3113560
C	51	-0.6002390	-1.9478770	-2.7458000
C	52	0.0490910	-0.8313980	-3.4060230
C	53	-3.3415700	1.1029310	-0.1862440
C	54	-2.3953410	2.1380610	-0.8114930
C	55	-1.8237820	-1.7759250	-2.0701640
C	56	-0.5379070	0.4349670	-3.3581710
C	57	-3.3481200	-0.1999760	-0.9749680
C	58	-1.7749490	1.9416940	-2.0304560
C	59	-2.4288050	-0.4501590	-2.0601520
C	60	-1.7875700	0.6160380	-2.6771740
C	61	-4.7777280	1.5359100	0.0794120
C	62	-5.7265240	0.5606350	0.3751800
C	63	-5.4796360	-0.7946550	0.2107940
C	64	-4.2998430	-1.2611420	-0.5762040
H	65	-4.9821900	2.5929720	0.2127140
H	66	-6.6891720	0.8732190	0.7746820
H	67	-6.2064960	-1.5365900	0.5267420
H	68	-4.6111200	-1.9058160	-1.4055760

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C	1	-4.034271	1.038467	2.557709
C	2	-4.645096	-0.140472	2.124466
C	3	-4.019974	2.211914	1.695313
C	4	-5.262955	-0.197723	0.811478
C	5	-2.764206	0.981323	3.254700
C	6	-4.013321	-1.423294	2.380035
C	7	-4.615463	2.154938	0.432755
C	8	-5.242798	0.925232	-0.019363
C	9	-2.145325	-0.248383	3.484177
C	10	-2.787369	-1.476624	3.047440
C	11	-2.747452	2.885773	1.869370
C	12	-5.015976	-1.517181	0.256683
C	13	-1.967712	2.115723	2.825256
C	14	-4.247711	-2.277054	1.226608
C	15	-3.952515	2.765228	-0.706772
C	16	-4.970016	0.775085	-1.438507
C	17	-0.714813	-0.395676	3.277435
C	18	-1.750793	-2.384079	2.588455
C	19	-2.115402	3.486343	0.775482
C	20	-4.757126	-1.664658	-1.108170
C	21	-0.596893	1.960815	2.627151
C	22	-3.253600	-3.157806	0.795029
C	23	-2.729553	3.411377	-0.538132
C	24	-4.728653	-0.492523	-1.973129
C	25	0.052979	0.684631	2.835922
C	26	-1.980728	-3.212158	1.492157
C	27	-4.164993	1.907852	-1.862366
C	28	-0.474075	-1.701889	2.727402
C	29	-0.681747	3.362045	0.601898
C	30	-3.725525	-2.579910	-1.555084
C	31	0.055328	2.602219	1.512207
C	32	-2.989227	-3.319397	-0.624969
C	33	-3.141220	1.726135	-2.792770
C	34	0.515427	-1.854600	1.752213
C	35	-1.664764	3.212097	-1.507600

C	36	-3.674759	-0.680069	-2.950363
C	37	1.120331	0.528458	1.848694
C	38	-0.934479	-3.418182	0.505447
C	39	-0.402298	3.185303	-0.808029
C	40	-3.056259	-1.971741	-2.694244
C	41	1.171249	1.809723	1.078690
C	42	-1.556046	-3.486359	-0.797440
C	43	-1.857758	2.383636	-2.604324
C	44	-2.886398	0.408920	-3.341202
C	45	1.317352	-0.739900	1.308411
C	46	0.300232	-2.768539	0.642548
C	47	0.667755	2.378464	-1.222610
C	48	-1.681442	-2.122742	-2.847397
C	49	1.650604	1.951019	-0.223160
C	50	-0.912903	-2.897888	-1.890503
C	51	-0.801895	1.468277	-3.003067
C	52	-1.453903	0.259872	-3.484161
C	53	1.974472	-1.152985	-0.078125
C	54	1.017136	-2.268387	-0.495422
C	55	0.434280	1.425766	-2.324524
C	56	-0.870331	-0.986298	-3.248947
C	57	2.016617	-0.049332	-1.108917
C	58	0.378632	-2.264328	-1.723465
C	59	1.045639	0.097946	-2.128296
C	60	0.378723	-1.057709	-2.566437
C	61	3.398636	-1.512833	0.318680
C	62	4.303375	-0.465607	0.487259
C	63	4.003204	0.838348	0.122208
C	64	2.824234	1.150055	-0.755844
H	65	3.625320	-2.529221	0.622589
H	66	5.262955	-0.672836	0.956528
H	67	4.689987	1.648209	0.349838
H	68	3.186829	1.652115	-1.664261

TS8

68

C	1	2.4874610	1.0169700	-2.6919930
C	2	3.1437340	-0.1370140	-2.2529630
C	3	2.4865570	2.2134620	-1.8604120
C	4	3.8161380	-0.1454310	-0.9682780
C	5	1.1938630	0.9164240	-3.3324910
C	6	2.5274170	-1.4388880	-2.4455280
C	7	3.1343370	2.2024480	-0.6233240
C	8	3.8082880	0.9990180	-0.1652010
C	9	0.5855290	-0.3339560	-3.4973670
C	10	1.2751090	-1.5358050	-3.0549310
C	11	1.1941890	2.8577990	-1.9979980
C	12	3.6235140	-1.4552110	-0.3683730
C	13	0.3925030	2.0445220	-2.8992350
C	14	2.8328120	-2.2582530	-1.2832880
C	15	2.5063610	2.8294780	0.5269490
C	16	3.5977540	0.8815600	1.2659470
C	17	-0.8251120	-0.5047130	-3.2294590
C	18	0.2831420	-2.4561820	-2.5301510
C	19	0.5970590	3.4763020	-0.8951640
C	20	3.4268710	-1.5713490	1.0094520
C	21	-0.9656210	1.8718950	-2.6427000
C	22	1.8830020	-3.1533860	-0.7879010
C	23	1.2651210	3.4471730	0.3932920
C	24	3.4076410	-0.3777550	1.8447290
C	25	-1.6042830	0.5741610	-2.7835790
C	26	0.5827700	-3.2563460	-1.4273670
C	27	2.7848570	2.0064910	1.6936460
C	28	-1.0128760	-1.8080800	-2.6303780
C	29	-0.8255660	3.3247440	-0.6579970
C	30	2.4384990	-2.4994490	1.5237410
C	31	-1.5811590	2.5332440	-1.5236280
C	32	1.6833270	-3.2820500	0.6459740
C	33	1.8024620	1.8268900	2.6686060
C	34	-1.9589910	-1.9707060	-1.6235640

C	35	0.2439020	3.2498260	1.4099110
C	36	2.4005570	-0.5617440	2.8675140
C	37	-2.6306740	0.4373650	-1.7698770
C	38	-0.4121320	-3.4592640	-0.3955250
C	39	-1.0422330	3.1797090	0.7660300
C	40	1.8027920	-1.8741050	2.6729190
C	41	-2.6547960	1.7182980	-1.0203850
C	42	0.2624720	-3.4765320	0.8831470
C	43	0.4988760	2.4506240	2.5171250
C	44	1.6013230	0.5196850	3.2632400
C	45	-2.8262270	-0.8626590	-1.1972640
C	46	-1.6672780	-2.8358890	-0.5011420
C	47	-2.0787440	2.3582150	1.2463240
C	48	0.4403760	-2.0525110	2.8891960
C	49	-3.0782810	1.8871160	0.2974880
C	50	-0.3467930	-2.8737310	1.9885290
C	51	-0.5188060	1.5215930	2.9809350
C	52	0.1820060	0.3426380	3.4689700
C	53	-3.2855520	-1.2125180	0.2634760
C	54	-2.3363910	-2.3171810	0.6559660
C	55	-1.7848980	1.4358380	2.3628020
C	56	-0.3825460	-0.9234330	3.2931380
C	57	-3.3913020	-0.1155060	1.2685750
C	58	-1.6558650	-2.2685100	1.8595590
C	59	-2.3831190	0.0891190	2.2404700
C	60	-1.6551180	-1.0409270	2.6686580
C	61	-4.5306750	-1.4868600	-0.5304050
C	62	-5.5328060	-0.4698270	-0.6112020
C	63	-5.3732770	0.7466110	-0.0260480
C	64	-4.2154160	1.0637190	0.8780150
H	65	-4.6987240	-2.4823690	-0.9241450
H	66	-6.4125740	-0.6690980	-1.2177360
H	67	-6.1187290	1.5244600	-0.1642170
H	68	-4.5864710	1.5839940	1.7708860

TS9

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C	1	-2.7116740	1.6374660	2.1626910
C	2	-3.3273520	0.3851420	1.9947930
C	3	-2.6434360	2.5681070	1.0599250
C	4	-3.8962710	0.0306360	0.7086490
C	5	-1.4666590	1.7322780	2.9074970
C	6	-2.7314330	-0.7997980	2.5675640
C	7	-3.1851240	2.2223440	-0.1869110
C	8	-3.8208680	0.9251970	-0.3621670
C	9	-0.8791880	0.5872800	3.4424920
C	10	-1.5242460	-0.7075770	3.2803200
C	11	-1.3595340	3.2543910	1.1240770
C	12	-3.6598960	-1.3862100	0.4862910
C	13	-0.6341510	2.7328110	2.2694150
C	14	-2.9358210	-1.8984300	1.6372880
C	15	-2.4717950	2.5421830	-1.4019740
C	16	-3.5019400	0.4415580	-1.6922280
C	17	0.5584640	0.3890120	3.3450370
C	18	-0.4902240	-1.6929060	3.0885180
C	19	-0.6794760	3.5783070	-0.0518850
C	20	-3.3575250	-1.8532220	-0.7933770
C	21	0.7450690	2.5305630	2.1816980
C	22	-1.9445240	-2.8631840	1.4603920
C	23	-1.2381740	3.2077760	-1.3393440
C	24	-3.2710380	-0.9188080	-1.9071260
C	25	1.3659080	1.3357960	2.7061960
C	26	-0.6906510	-2.7576280	2.1960980
C	27	-2.6477710	1.4351570	-2.3278500
C	28	0.7984280	-1.0083000	3.1244620
C	29	0.7604440	3.4041600	-0.1231110
C	30	-2.3284770	-2.8611910	-0.9773390
C	31	1.4466830	2.8896960	0.9779280
C	32	-1.6373030	-3.3583150	0.1322680
C	33	-1.5922420	1.0211320	-3.1390900
C	34	1.8291420	-1.3915560	2.2615540
C	35	-0.1446570	2.7705280	-2.1722240

C	36	-2.1876680	-1.3500180	-2.7679680
C	37	2.4732210	0.9403620	1.8335540
C	38	0.3753320	-3.1987160	1.3426810
C	39	1.0878480	2.8935980	-1.4368560
C	40	-1.6132920	-2.5498140	-2.2013270
C	41	2.5642970	2.0104800	0.7874250
C	42	-0.1983510	-3.5616540	0.0613150
C	43	-0.2958800	1.6869620	-3.0435800
C	44	-1.3542490	-0.3854930	-3.3672150
C	45	2.6993410	-0.4239350	1.6269650
C	46	1.6256840	-2.5318250	1.3754060
C	47	2.1641550	2.0094380	-1.6079570
C	48	-0.2290230	-2.7541430	-2.2637070
C	49	3.0809790	1.8408270	-0.4924820
C	50	0.4853730	-3.2724050	-1.1188680
C	51	0.7481040	0.7125630	-3.1795910
C	52	0.0757270	-0.5794960	-3.3907380
C	53	3.2849530	-1.1276210	0.3615320
C	54	2.3486330	-2.3016850	0.1879310
C	55	1.9803920	0.8118060	-2.4689350
C	56	0.6205080	-1.7458880	-2.8707680
C	57	3.4851770	-0.3349330	-0.8957800
C	58	1.7870850	-2.6124990	-1.0575920
C	59	2.5763130	-0.4327590	-1.9922450
C	60	1.8517240	-1.6679250	-2.1323280
C	61	4.7467790	-1.4655410	0.2032150
C	62	5.7127050	-0.4498370	0.5185500
C	63	5.3983790	0.8230860	0.1802660
C	64	4.2492300	0.9425000	-0.7705070
H	65	5.0207220	-2.4880630	-0.0362210
H	66	6.6555460	-0.7184350	0.9900430
H	67	6.0010800	1.6897760	0.4305640
H	68	4.6656710	1.2177350	-1.7499070

3a (T)

68

C	1	-2.7348410	2.0561170	1.7351420
C	2	-3.3655240	0.7953510	1.8019980
C	3	-2.6273980	2.7443040	0.4802240
C	4	-3.9106820	0.1969970	0.5922500
C	5	-1.5054810	2.2898520	2.4851920
C	6	-2.7996930	-0.2498370	2.6050640
C	7	-3.1500360	2.1640780	-0.6944860
C	8	-3.8009700	0.8620910	-0.6276180
C	9	-0.9477100	1.2725720	3.2520560
C	10	-1.6049540	-0.0259070	3.3256040
C	11	-1.3350390	3.4219650	0.4430780
C	12	-3.6914780	-1.2372800	0.6585350
C	13	-0.6436690	3.1393550	1.6903740
C	14	-2.9986680	-1.5147800	1.9032360
C	15	-2.4056150	2.2281050	-1.9191880
C	16	-3.4610660	0.1213850	-1.8302630
C	17	0.4908180	1.0530830	3.2417070
C	18	-0.5852120	-1.0294490	3.3538880
C	19	-0.6231230	3.5015640	-0.7514680
C	20	-3.3676520	-1.9539120	-0.4970630
C	21	0.7361720	2.9167290	1.6853740
C	22	-2.0195660	-2.5023880	1.9473500
C	23	-1.1578050	2.8820760	-1.9554260
C	24	-3.2454140	-1.2591290	-1.7691640
C	25	1.3338790	1.8494940	2.4567000
C	26	-0.7813780	-2.2602020	2.6830120
C	27	-2.5779980	0.9591290	-2.6208880
C	28	0.7114790	-0.3623560	3.2965310
C	29	0.8160670	3.3070620	-0.7461000
C	30	-2.3482550	-2.9853970	-0.4509550
C	31	1.4746620	3.0226950	0.4549360
C	32	-1.6883030	-3.2566950	0.7536310
C	33	-1.5114430	0.3837490	-3.3086970
C	34	1.7558650	-0.9106890	2.5515650
C	35	-0.0591270	2.2715670	-2.6400320

C	36	-2.1465250	-1.8574770	-2.5011000
C	37	2.4624700	1.2877040	1.7090930
C	38	0.2897170	-2.8557380	1.9620680
C	39	1.1564810	2.5259760	-1.9085660
C	40	-1.5970250	-2.9265000	-1.6903060
C	41	2.5909890	2.1270550	0.4766710
C	42	-0.2521110	-3.4733350	0.7608730
C	43	-0.2034110	1.0359370	-3.2974470
C	44	-1.2908460	-1.0412950	-3.2549190
C	45	2.6791040	-0.1015700	1.7739000
C	46	1.5448390	-2.1938260	1.8925830
C	47	2.2229660	1.6168100	-1.8646130
C	48	-0.2139620	-3.1442790	-1.6752090
C	49	3.1247090	1.6932240	-0.7396260
C	50	0.4674840	-3.4255080	-0.4314700
C	51	0.8166170	0.0465570	-3.2022020
C	52	0.1444740	-1.2477200	-3.2013220
C	53	3.2017350	-1.0266160	0.6803700
C	54	2.2823310	-2.1904940	0.6994490
C	55	2.0451030	0.2622230	-2.4706440
C	56	0.6644190	-2.2887580	-2.4507690
C	57	3.6510610	-0.5994940	-0.7497590
C	58	1.7786560	-2.7790440	-0.4759280
C	59	2.6426230	-0.8697690	-1.8130850
C	60	1.8995250	-2.0837140	-1.7251900
C	61	4.5982940	-1.3917760	0.1511290
C	62	5.6731020	-0.4470160	0.5669270
C	63	5.4432120	0.7853240	0.1043340
C	64	4.2883070	0.7796370	-0.8604100
H	65	4.7931590	-2.4535090	0.0312890
H	66	6.4795150	-0.7477290	1.2279190
H	67	6.0274910	1.6738870	0.3167940
H	68	4.6887630	0.8804490	-1.8815700

4a (T)

68

C	1	3.742035	-2.775055	0.764359
C	2	4.359146	-1.723190	1.448837
C	3	3.744186	-2.791122	-0.690308
C	4	5.003952	-0.650925	0.712753
C	5	2.457000	-3.279083	1.213287
C	6	3.709457	-1.127335	2.604462
C	7	4.363358	-1.755310	-1.395981
C	8	5.006775	-0.666763	-0.681915
C	9	1.829010	-2.697845	2.322449
C	10	2.470657	-1.599731	3.022552
C	11	2.459885	-3.304779	-1.132065
C	12	4.770386	0.596893	1.426315
C	13	1.668808	-3.605591	0.043700
C	14	3.970734	0.306824	2.587982
C	15	3.718216	-1.186661	-2.567520
C	16	4.775284	0.564484	-1.423248
C	17	0.409119	-2.421219	2.289581
C	18	1.434433	-0.653946	3.415924
C	19	1.836792	-2.750320	-2.255585
C	20	4.568665	1.789566	0.708969
C	21	0.293808	-3.346420	0.038925
C	22	2.974457	1.208800	2.999054
C	23	2.480286	-1.668747	-2.978943
C	24	4.571060	1.772858	-0.733322
C	25	-0.354553	-2.751312	1.180237
C	26	1.683670	0.726624	3.409149
C	27	3.978073	0.247681	-2.580673
C	28	0.186111	-1.136871	2.953033
C	29	0.415497	-2.470856	-2.232391
C	30	3.557663	2.737152	1.150696
C	31	-0.346909	-2.773422	-1.115600
C	32	2.771469	2.448593	2.267700
C	33	2.982971	1.139694	-3.013809
C	34	-0.859055	-0.285172	2.524750
C	35	1.444855	-0.731949	-3.394287

C	36	3.560684	2.710403	-1.198792
C	37	-1.460663	-1.896088	0.740112
C	38	0.657104	1.634018	2.927826
C	39	0.193161	-1.205017	-2.924164
C	40	2.946838	3.319275	-0.031540
C	41	-1.452896	-1.904846	-0.696320
C	42	1.347305	2.725113	2.251282
C	43	1.692627	0.646851	-3.415924
C	44	2.777588	2.395660	-2.311066
C	45	-1.856171	-0.809479	1.645935
C	46	-0.606873	1.179779	2.495941
C	47	-0.853622	-0.345398	-2.519714
C	48	1.585297	3.605606	-0.036865
C	49	-1.847809	-0.848724	-1.619781
C	50	0.775452	3.314514	1.130386
C	51	0.664566	1.564636	-2.956757
C	52	1.352844	2.671036	-2.304153
C	53	-2.305069	1.247086	0.674896
C	54	-1.256027	1.909668	1.399536
C	55	-0.600311	1.120056	-2.517944
C	56	0.778717	3.287308	-1.199081
C	57	-2.303268	1.232712	-0.702057
C	58	-0.524887	2.877502	0.693130
C	59	-1.252457	1.876709	-1.440613
C	60	-0.522751	2.860550	-0.755432
C	61	-3.025421	0.132462	1.414886
C	62	-4.188019	-0.455902	0.668869
C	63	-4.183746	-0.473541	-0.660477
C	64	-3.019028	0.099442	-1.414902
H	65	-3.355331	0.495041	2.395508
H	66	-5.006790	-0.874252	1.247818
H	67	-4.997772	-0.908676	-1.233688
H	68	-3.345535	0.436020	-2.405762

TS (from 15 to 2a)

68

C	1	-2.4339040	-0.6496140	2.8315490
C	2	-3.1152500	-1.3630330	1.8407920
C	3	-2.4207390	0.8100230	2.7977180
C	4	-3.8001110	-0.6550680	0.7771920
C	5	-1.1437980	-1.1019460	3.2997960
C	6	-2.5151020	-2.5589660	1.2721110
C	7	-3.0911400	1.4888530	1.7743010
C	8	-3.7870880	0.7450200	0.7448320
C	9	-0.5592920	-2.2543740	2.7510230
C	10	-1.2666160	-2.9940330	1.7159570
C	11	-1.1233460	1.2592800	3.2439630
C	12	-3.6244800	-1.4098000	-0.4501030
C	13	-0.3259580	0.0774120	3.5385820
C	14	-2.8334500	-2.5883310	-0.1462620
C	15	-2.4693170	2.6460730	1.1496570
C	16	-3.6001970	1.4399110	-0.5171790
C	17	0.8478710	-2.2825440	2.4405110
C	18	-0.2840310	-3.4724130	0.7588300
C	19	-0.5166510	2.3757180	2.6406390
C	20	-3.4426030	-0.7414730	-1.6648450
C	21	1.0272770	0.0586780	3.2260770
C	22	-1.8918730	-3.0558300	-1.0651110
C	23	-1.2129310	3.0769870	1.5713680
C	24	-3.4308900	0.7134960	-1.6992680
C	25	1.6373000	-1.1333040	2.6640000
C	26	-0.5908620	-3.5053370	-0.6022930
C	27	-2.7895430	2.6174290	-0.2686450
C	28	1.0217160	-3.0231080	1.2050270
C	29	0.8875810	2.3698310	2.3334460
C	30	-2.4609220	-1.2218630	-2.6156230
C	31	1.6595280	1.2156860	2.6076420
C	32	-1.6995110	-2.3573660	-2.3255330
C	33	-1.8431200	3.0289410	-1.2086540
C	34	1.9732990	-2.6122590	0.2697780
C	35	-0.2249500	3.4964730	0.5927700

C	36	-2.4425930	1.1336870	-2.6719830
C	37	2.6280790	-0.7108400	1.7257180
C	38	0.3982760	-3.0833310	-1.5764800
C	39	1.0747100	3.0516460	1.0555020
C	40	-1.8351430	-0.0626700	-3.2327220
C	41	2.6506790	0.7500320	1.7067130
C	42	-0.2818040	-2.3790420	-2.6356130
C	43	-0.5341620	3.4796150	-0.7679910
C	44	-1.6622870	2.2691380	-2.4344450
C	45	2.8587580	-1.4782200	0.5484110
C	46	1.6524270	-2.6267260	-1.1394260
C	47	2.0259950	2.6043040	0.1485250
C	48	-0.4711450	-0.0805400	-3.5215760
C	49	2.9831400	1.5064890	0.4999970
C	50	0.3237970	-1.2581590	-3.2182480
C	51	0.4474350	2.9952510	-1.7157750
C	52	-0.2451740	2.2536870	-2.7435140
C	53	3.2094890	-0.8149830	-0.7942500
C	54	2.2932880	-1.5080440	-1.7787330
C	55	1.6973610	2.5448290	-1.2538050
C	56	0.3411090	1.0970350	-3.2718490
C	57	3.2064420	0.7111940	-0.8438560
C	58	1.6263930	-0.8200830	-2.7725560
C	59	2.3064340	1.3743930	-1.8348270
C	60	1.6356770	0.6591400	-2.8054750
C	61	4.4734810	-1.4749380	-0.3463480
C	62	5.5401580	-0.6885740	0.2003610
C	63	5.4978170	0.6723800	0.2651690
C	64	4.3707660	1.4572170	-0.2554950
H	65	4.6567450	-2.4996350	-0.6493420
H	66	6.4191190	-1.2142970	0.5634940
H	67	6.3414170	1.2208890	0.6744250
H	68	4.6249280	2.4148340	-0.7054040

2a(T)

68

C	1	-2.3588250	-0.7495750	2.8522030
C	2	-3.0599050	-1.4395730	1.8550950
C	3	-2.3585430	0.7132390	2.8611810
C	4	-3.7702930	-0.7075810	0.8309490
C	5	-1.0614650	-1.2051580	3.2800540
C	6	-2.4625970	-2.6148740	1.2379690
C	7	-3.0596260	1.4158800	1.8727890
C	8	-3.7703470	0.6970500	0.8398280
C	9	-0.4761960	-2.3392360	2.6833180
C	10	-1.2015880	-3.0502750	1.6400920
C	11	-1.0613110	1.1630870	3.2945380
C	12	-3.6178680	-1.4238180	-0.4226120
C	13	-0.2471430	-0.0226260	3.5329210
C	14	-2.8124540	-2.6056680	-0.1729980
C	15	-2.4624800	2.5989810	1.2705330
C	16	-3.6179940	1.4291900	-0.4048070
C	17	0.9182150	-2.3491400	2.3444700
C	18	-0.2376530	-3.4934810	0.6475410
C	19	-0.4756570	2.3043820	2.7116060
C	20	-3.4679330	-0.7181930	-1.6198810
C	21	1.0938930	-0.0206260	3.1918490
C	22	-1.8892470	-3.0394070	-1.1260220
C	23	-1.2012660	3.0290080	1.6778130
C	24	-3.4681180	0.7387340	-1.6108160
C	25	1.7061560	-1.1919200	2.5824690
C	26	-0.5744270	-3.4930100	-0.7055470
C	27	-2.8127580	2.6078780	-0.1403840
C	28	1.0750120	-3.0510000	1.0761430
C	29	0.9182740	2.3181590	2.3728580
C	30	-2.5054270	-1.1620480	-2.6063850
C	31	1.7069640	1.1580040	2.5967220
C	32	-1.7279230	-2.3001010	-2.3662640
C	33	-1.8896160	3.0536060	-1.0880730
C	34	2.0127410	-2.6246880	0.1442060
C	35	-0.2376420	3.4849870	0.6909650

C	36	-2.5056270	1.1950760	-2.5918360
C	37	2.6755000	-0.7451790	1.6555410
C	38	0.3920660	-3.0307220	-1.6810220
C	39	1.0750340	3.0367380	1.1135790
C	40	-1.9019890	0.0202420	-3.2003410
C	41	2.6759220	0.7223510	1.6650270
C	42	-0.3176190	-2.3011680	-2.7056690
C	43	-0.5748370	3.5020700	-0.6620510
C	44	-1.7285180	2.3301990	-2.3377220
C	45	2.9870820	-1.5316110	0.4652430
C	46	1.6555870	-2.5845910	-1.2526990
C	47	2.0116670	2.6216010	0.1761460
C	48	-0.5442910	0.0223650	-3.5176790
C	49	2.9860920	1.5223390	0.4810650
C	50	0.2644780	-1.1570880	-3.2642720
C	51	0.3913480	3.0525900	-1.6436290
C	52	-0.3179330	2.3356490	-2.6772650
C	53	3.1869260	-0.7477270	-0.9124500
C	54	2.2609120	-1.4279650	-1.8651000
C	55	1.6546630	2.6002920	-1.2208530
C	56	0.2643540	1.1987530	-3.2503260
C	57	3.1849590	0.7613160	-0.9003990
C	58	1.5698810	-0.7211560	-2.8288370
C	59	2.2604760	1.4523380	-1.8482540
C	60	1.5700780	0.7572000	-2.8202760
C	61	4.3478490	-1.4834020	-0.3086500
C	62	5.4659280	-0.6734350	0.2168070
C	63	5.4668900	0.6722950	0.2249510
C	64	4.3487120	1.4895570	-0.2889620
H	65	4.6186620	-2.4396250	-0.7515980
H	66	6.3289650	-1.2148590	0.5954220
H	67	6.3309520	1.2080080	0.6091290
H	68	4.6181600	2.4517750	-0.7193100