

## Supporting Information for

### Nitrenium ions and trivalent boron ligands as analogues of N-heterocyclic carbenes in olefin metathesis; a computational study

A. Pazio,<sup>ab</sup> K. Woźniak,<sup>b</sup> K. Grela<sup>b</sup> and B. Trzaskowski\*<sup>a</sup>

<sup>a</sup> Centre of New Technologies, University of Warsaw, Banacha 2c, 02-097 Warszawa, Poland

<sup>b</sup> Biological and Chemical Research Centre, Department of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warszawa, Poland

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## Geometry comparison of investigated structures

### Numeric values

**Table S1.** Geometry comparison amongst **2** structures (triazolium derivatives; **NHNs**). **1** stands for two types of Hoveyda catalyst's structures: from the **X-ray** measurement and DFT-**optimized**.

	<b>1 X-ray<sup>1</sup></b>	<b>1 opt</b>	<b>2a</b>	<b>2b</b>	<b>2c</b>			
Ru(1)-C(22)	1.829(1)	1.832	1.846	1.848	1.850	Ru center	Bond length (Å)	
Ru(1)-C(1)	1.979(1)	1.972	2.052	2.033	2.010			
Ru(1)-Cl(1)	2.3379(5)	2.404	2.389	2.385	2.385			
Ru(1)-Cl(2)	2.3278(5)	2.392	2.392	2.389	2.388			
Ru(1)-O(1)	2.256(1)	2.322	2.188	2.183	2.192			
C(4)-C(22) distance	3.072(2)	3.188	3.157	3.160	3.134			
O(1)-C(28)	1.370(2)	1.352	1.359	1.359	1.358	O atom		
O(1)-C(29)	1.469(2)	1.449	1.469	1.471	1.471			
N(1)-C(4)	1.434(2)	1.432	1.437	1.439	1.434	NHC		
N(2)-C(13)	1.439(2)	1.442	1.440	1.441	1.437			
C(2)-C(3)	1.524(2)	1.516	1.371	1.360	1.375			
C(2)-N(1)	1.472(2)	1.475	1.372	1.363	1.370			
C(3)-N(2)	1.474(2)	1.476	1.367	1.359	1.391			
N(3)-N(1)	1.351(2)	1.352	1.331	1.334	1.337			
N(3)-N(2)	1.352(2)	1.354	1.336	1.340	1.343			
N(1)-C(1)/N(3)-N(2)	107.2(1)	106.77	104.34	104.50	105.86	NHC / ADC	Plane angles (°)	
C(1)/N(3)-N(1)-C(4)	126.9(1)	126.77	122.88	123.78	124.34			
C(1)/N(3)-N(1)-C(13)	126.6(1)	126.73	120.43	121.01	121.27			
C(1)/N(3)-N(1)-C(2)	113.6(1)	113.83	112.17	111.56	111.16			
C(1)/N(3)-N(2)-C(3)	113.5(1)	113.42	112.33	111.74	111.40			
C(1)/N(3)-Ru(1)-C(22)	101.34(6)	103.10	102.54	102.34	102.28			
Cl(1)-Ru(1)-Cl(2)	156.25(1)	160.20	163.40	163.37	163.30	Ru center		
Ru(1)-C(22)-C(23)	118.5(1)	119.10	117.98	117.84	117.99			
C(22)-C(23)-C(28)	118.5(1)	119.32	117.64	117.63	117.71			
Ru(1)-C(1)-N(1)-C(2)	-173.3(1)	-178.09	177.97	176.42	177.42	NHC / ADC		Torsion angles (°)
Ru(1)-C(1)-N(2)-C(3)	171.0(1)	-178.58	-178.29	-177.02	-177.87			
Ru(1)-C(1)-N(1)-C(4)	17.7(2)	-10.81	-3.64	-5.76	-4.94			
Ru(1)-C(1)-N(2)-C(13)	-22.4(2)	13.67	3.24	4.45	4.09			
C(4)-N(1)-Ru(1)-C(22)	-2.91(9)	-3.52	-0.04	-0.83	-0.51			
C(22)-Ru(1)-O(1)-C(28)	7.1(1)	-1.66	3.17	2.66	2.91	benzylidene		
Ru(1)-C(22)-C(23)-C(28)	4.1(2)	-2.26	2.58	2.18	2.27			
C(22)-C(23)-C(28)-O(1)	2.7(2)	0.55	0.39	0.31	0.46			
O(1)-Ru(1)-C(22)-C(23)	-5.8(1)	1.99	-2.98	-2.51	-2.68			
C(1)-Ru(1)-O(1)-C(29)	90.4(8)	-51.84	7.18	-6.79	-4.40			

**Table S2.** Geometry comparison amongst **9** structures (boryl derivatives; **NHBs**). **1** stands for two types of Hoveyda catalyst's structures: from the **X-ray** measurement and DFT-**optimized**.

	<b>1 X-ray</b>	<b>1 opt</b>	<b>9a</b>	<b>9b</b>	<b>9c</b>		
Ru(1)-C(22)	1.829(1)	1.832	1.823	1.824	1.824	Ru center	Bond length (Å)
Ru(1)-C(1)/B(1)	1.979(1)	1.972	2.016	2.023	2.002		
Ru(1)-Cl(1)	2.3379(5)	2.404	2.384	2.387	2.385		
Ru(1)-Cl(2)	2.3278(5)	2.392	2.408	2.409	2.406		
Ru(1)-O(1)	2.256(1)	2.322	2.540	2.546	2.526		
C(4)-C(22) distance	3.072(2)	3.188	3.249	3.237	3.246		
O(1)-C(28)	1.370(2)	1.352	1.350	1.349	1.349	O atom	
O(1)-C(29)	1.469(2)	1.449	1.430	1.430	1.431		

<sup>1</sup> REFCODE: ABEJUM01 CSD ver. 5.35 Nov 2013

N(1)-C(4)	1.434(2)	1.432	1.416	1.415	1.417	NHC	
N(2)-C(13)	1.439(2)	1.442	1.420	1.420	1.422		
C(2)-C(3)	1.524(2)	1.516	1.348	1.356	1.409		
C(2)-N(1)	1.472(2)	1.475	1.401	1.411	1.391		
C(3)-N(2)	1.474(2)	1.476	1.398	1.409	1.388		
C(1)/B(1)-N(1)	1.351(2)	1.352	1.469	1.466	1.476		
C(1)/B(1)-N(2)	1.352(2)	1.354	1.472	1.469	1.479		
N(1)-C(1)/B(1)-N(2)	107.2(1)	106.77	101.68	101.67	102.32	NHC	Plane angles (°)
C(1)/B(1)-N(1)-C(4)	126.9(1)	126.77	130.21	128.77	129.72		
C(1)/B(1)-N(1)-C(13)	126.6(1)	126.73	129.93	128.33	129.05		
C(1)/B(1)-N(1)-C(2)	113.6(1)	113.83	109.71	110.12	110.07		
C(1)/B(1)-N(2)-C(3)	113.5(1)	113.42	109.67	110.10	110.12		
C(1)/B(1)-Ru(1)-C(22)	101.34(6)	103.10	98.90	99.59	99.48		
Cl(1)-Ru(1)-Cl(2)	156.25(1)	160.20	149.45	150.03	150.34	Ru center	
Ru(1)-C(22)-C(23)	118.5(1)	119.10	122.30	122.50	121.97		
C(22)-C(23)-C(28)	118.5(1)	119.32	121.44	121.47	121.37		
Ru(1)-C(1)/B(1)-N(1)-C(2)	-173.3(1)	-178.09	175.70	177.51	175.51	NHC	Torsion angles (°)
Ru(1)-C(1)/B(1)-N(2)-C(3)	171.0(1)	-178.58	-175.96	-177.66	-175.76		
Ru(1)-C(1)/B(1)-N(1)-C(4)	17.7(2)	-10.81	-16.26	-12.34	-11.45		
Ru(1)-C(1)/B(1)-N(2)-C(13)	-22.4(2)	13.67	15.91	14.11	13.12		
C(4)-N(1)-Ru(1)-C(22)	-2.91(9)	-3.52	7.22	8.25	8.60		
C(22)-Ru(1)-O(1)-C(28)	7.1(1)	-1.66	-2.11	-1.50	-0.42	benzylidene	
Ru(1)-C(22)-C(23)-C(28)	4.1(2)	-2.26	0.21	0.38	1.41		
C(22)-C(23)-C(28)-O(1)	2.7(2)	0.55	-2.39	-1.92	-1.74		
O(1)-Ru(1)-C(22)-C(23)	-5.8(1)	1.99	1.00	0.59	-0.46		
C(1)/B(1)-Ru(1)-O(1)-C(29)	90.4(8)	-51.84	-143.40	-147.63	-146.52		

**Table S3.** Geometry comparison amongst **12** and **13** structures (backbone modifications of **2**). **1** stands for two types of Hoveyda catalyst's structures: from the **X-ray** measurement and DFT-optimized.

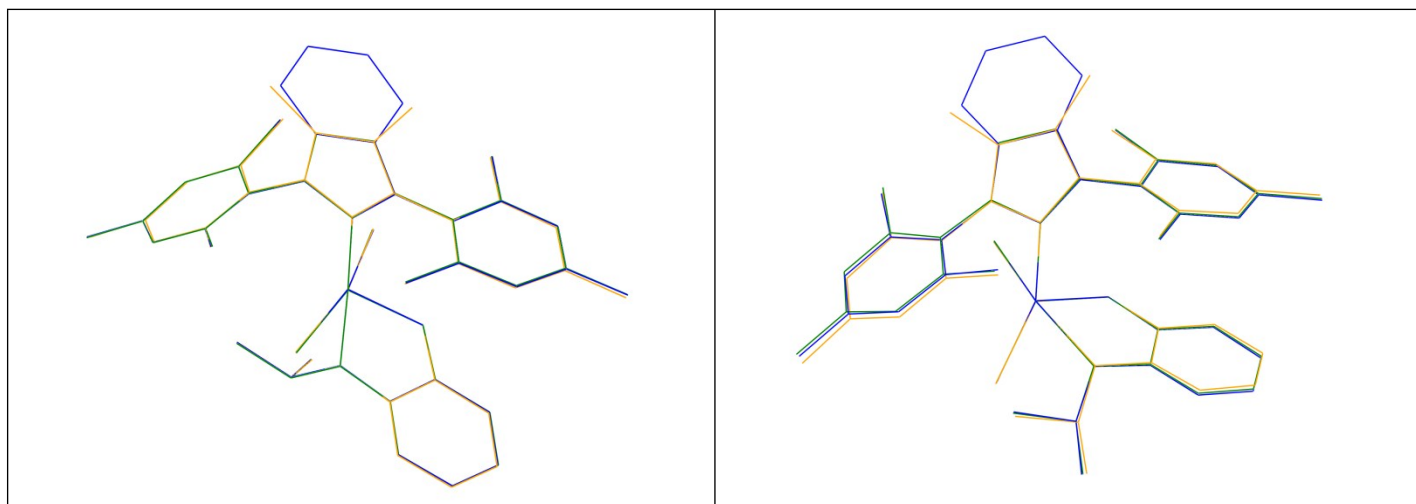
	<b>1 opt</b>	<b>12a</b>	<b>12b</b>	<b>13a</b>	<b>13b</b>		
Ru(1)-C(22)	1.832	1.831	1.830	1.832	1.831	Ru center	Bond length (Å)
Ru(1)-C(1)	1.972	2.103	2.108	2.099	2.101		
Ru(1)-Cl(1)	2.404	2.396	2.402	2.397	2.398		
Ru(1)-Cl(2)	2.392	2.399	2.393	2.401	2.402		
Ru(1)-O(1)	2.322	2.200	2.206	2.202	2.202		
C(4)-C(22) distance	3.188	3.189	3.194	3.191	3.190		
O(1)-C(28)	1.352	1.359	1.360	1.358	1.358		
O(1)-C(29)	1.449	1.458	1.457	1.460	1.460		
N(1)-C(4)	1.432	1.423	1.424	1.433	1.432	NHC	
N(2)-C(13)	1.442	1.436	1.438	1.427	1.427		
C(2)-C(3)	1.516	1.422	1.428	1.423	1.426		
C(2)-N(1)	1.475	1.433	1.416	1.351	1.352		
C(3)-N(2)	1.476	1.347	1.344	1.426	1.414		
N(3)-N(1)	1.352	1.347	1.352	1.316	1.322		
N(3)-N(2)	1.354	1.321	1.333	1.350	1.353		
N(1)-C(1)/N(3)-N(2)	106.77	104.05	103.84	104.15	103.89	NHC	Plane angles (°)
C(1)/N(3)-N(1)-C(4)	126.77	122.88	121.82	122.13	121.62		
C(1)/N(3)-N(1)-C(13)	126.73	120.13	119.72	120.59	120.53		
C(1)/N(3)-N(1)-C(2)	113.83	113.53	113.34	113.61	113.92		
C(1)/N(3)-N(2)-C(3)	113.42	113.90	113.96	113.76	113.61		
C(1)/N(3)-Ru(1)-C(22)	103.10	102.10	102.27	102.78	102.91		
Cl(1)-Ru(1)-Cl(2)	160.20	162.14	162.38	163.09	163.25	Ru center	
Ru(1)-C(22)-C(23)	119.10	118.02	118.24	118.17	118.17		
C(22)-C(23)-C(28)	119.32	117.74	117.72	117.65	117.64		
Ru(1)-C(1)-N(1)-C(2)	-178.09	178.30	153.86	-179.81	-179.73	NH ion	Torsion
Ru(1)-C(1)-N(2)-C(3)	-178.58	-178.61	-157.89	179.72	179.61		
Ru(1)-C(1)-N(1)-C(4)	-10.81	-2.78	-34.75	0.79	0.97		

Ru(1)-C(1)-N(2)-C(13)	13.67	1.53	25.70	1.85	1.99	benzylidene	es (°)
C(4)-N(1)-Ru(1)-C(22)	-3.52	0.31	-2.87	0.77	0.73		
C(22)-Ru(1)-O(1)-C(28)	-1.66	1.97	0.08	1.90	1.84	benzylidene	
Ru(1)-C(22)-C(23)-C(28)	-2.26	2.09	0.43	2.05	2.06		
C(22)-C(23)-C(28)-O(1)	0.55	-0.21	-0.34	-0.23	-0.30		
O(1)-Ru(1)-C(22)-C(23)	1.99	-2.10	-0.26	-2.04	-2.02		
C(1)-Ru(1)-O(1)-C(29)	-51.84	21.13	-31.85	21.10	20.40		

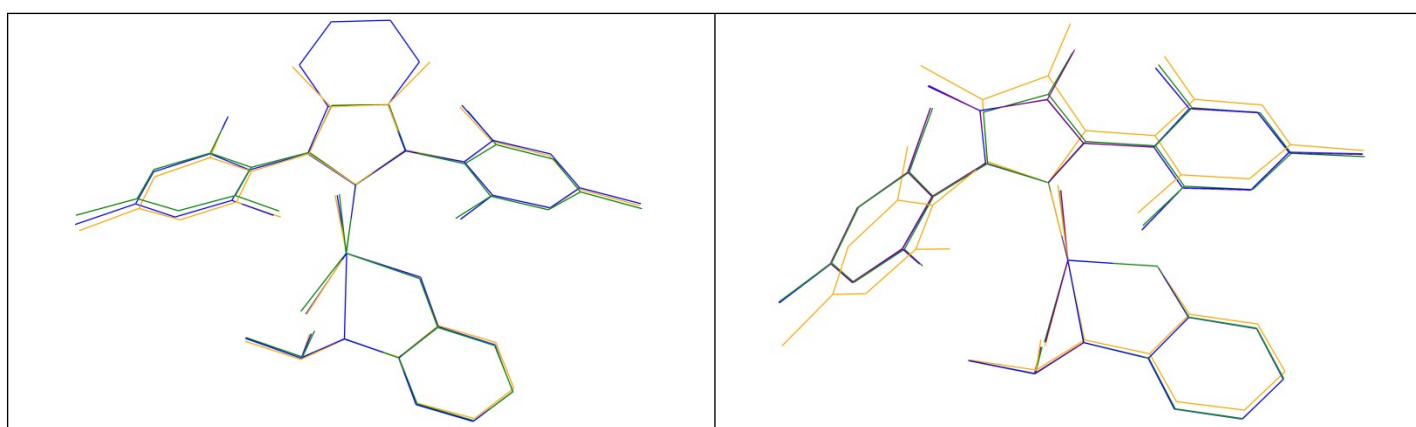
**Table S4.** The comparison of the geometry amongst all investigated compounds – type **a: 1** stands for two types of Hoveyda catalyst's structures: from the **X-ray** measurement and DFT-**optimized**.

	<b>1 X-ray X=C(1)</b>	<b>1 opt X=C(1)</b>	<b>2a X=N(3)</b>	<b>9a X=B(1)</b>	<b>12a X=N(3)</b>	<b>13a X=N(3)</b>		
Ru(1)-C(22)	1.829(1)	1.833	1.848	1.823	1.831	1.832	Ru center	Bond length (Å)
Ru(1)-X	1.979(1)	1.972	2.033	2.016	2.103	2.099		
Ru(1)-Cl(1)	2.3379(5)	2.396	2.386	2.384	2.396	2.397		
Ru(1)-Cl(2)	2.3278(5)	2.400	2.389	2.408	2.399	2.401		
Ru(1)-O(1)	2.256(1)	2.328	2.183	2.540	2.200	2.202		
C(4)-C(22) distance	3.072(2)	3.166	3.160	3.249	3.189	3.191		
O(1)-C(28)	1.370(2)	1.352	1.359	1.350	1.359	1.358	O	
O(1)-C(29)	1.469(2)	1.449	1.471	1.430	1.458	1.460		
N(1)-C(4)	1.434(2)	1.423	1.439	1.416	1.423	1.433	NHC	
N(2)-C(13)	1.439(2)	1.427	1.441	1.420	1.436	1.427		
C(2)-C(3)	1.524(2)	1.524	1.360	1.348	1.422	1.423		
C(2)-N(1)	1.472(2)	1.467	1.363	1.401	1.433	1.351		
C(3)-N(2)	1.474(2)	1.462	1.359	1.398	1.347	1.426		
X-N(1)	1.351(2)	1.352	1.334	1.469	1.347	1.316		
X-N(2)	1.352(2)	1.360	1.340	1.472	1.321	1.350		
N(1)-X-N(2)	107.2(1)	106.71	104.50	101.68	104.05	104.15	ADC	Plane angles (°)
X-N(1)-C(4)	126.9(1)	127.77	123.78	130.21	122.88	122.13		
X-N(1)-C(13)	126.6(1)	124.58	121.01	129.93	120.13	120.59		
X-N(1)-C(2)	113.6(1)	112.97	111.56	109.71	113.53	113.61		
X-N(1)-C(3)	113.5(1)	113.40	111.74	109.67	113.90	113.76		
X-Ru(1)-C(22)	101.34(6)	102.68	102.34	98.90	102.10	102.78		
Cl(1)-Ru(1)-Cl(2)	156.25(1)	160.26	163.37	149.45	162.14	163.09	Ru center	
Ru(1)-C(22)-C(23)	118.5(1)	119.3	117.8	122.30	118.02	118.17		
C(22)-C(23)-C(28)	118.5(1)	119.3	117.6	121.44	117.74	117.65		
Ru(1)-X-N(1)-C(2)	-173.3(1)	-174.13	176.42	175.70	178.30	-179.81	NHC	Torsion angles (°)
Ru(1)-X-N(1)-C(3)	171.0(1)	-174.91	-177.02	-175.96	-178.61	179.72		
Ru(1)-X-N(1)-C(4)	17.7(2)	3.48	-5.76	-16.26	-2.78	0.79		
Ru(1)-X-N(2)-C(13)	-22.4(2)	5.28	4.45	15.91	1.53	1.85		
C(4)-N(1)-Ru(1)-C(22)	-2.91(9)	1.60	-0.83	7.22	0.31	0.77		
C(22)-Ru(1)-O(1)-C(28)	7.1(1)	0.99	2.66	-2.11	1.97	1.90	benzylidene	
Ru(1)-C(22)-C(23)-C(28)	4.1(2)	1.56	2.18	0.21	2.09	2.05		
C(22)-C(23)-C(28)-O(1)	2.7(2)	-0.53	0.31	-2.39	-0.21	-0.23		
O(1)-Ru(1)-C(22)-C(23)	-5.8(1)	-1.30	-2.51	1.00	-2.10	-2.04		
X-Ru(1)-O(1)-C(29)	90.4(8)	18.36	-6.79	-143.40	21.13	21.10		

## Molecular overlays of investigated structures



**Figure S1.** Molecular overlay of investigated structures - catalyst **2a** (green), **2b** (orange) and **2c** (blue): *trans* (left) and *cis* (right).



**Figure S2.** Molecular overlay of investigated structures, catalyst **9** (left): **9a** (green), **9b** (orange) and **9c** (blue) and catalysts 12 and 13: **12a** (green), **12b** (orange) and **13a** (blue), **13b** (purple).

## Energy Values Tables

**Table S5.** Total energy values (E) and free energy values (G; as defined in the manuscript) for the initiation reaction following either the interchange or dissociative mechanism for **2a-c**. "S" stands for pre-catalyst, "TS" for transition state and "P" for product of the reaction (activated catalyst).

compound	structure	M06 Gas Phase, LACVP++ E (Hartrees)	solvation E in DCM (hartrees)	ZPE (kcal/mol)	S (cal/mol)	Thermal correction to enthalpy (kcal/mol)	G (Hartrees)
<b>2a</b>	S <i>trans</i>	-2417.761135	-0.056417	374.124	242.131	23.281	-2417.299234
	S <i>cis</i>	-2417.746187	-0.064781	374.501	234.568	22.930	-2417.289017
	TS interchange mechanism	-2574.873877	-0.053483	442.276	261.381	26.574	-2574.304329
	P interchange mechanism	-2574.906103	-0.054168	442.931	260.536	26.761	-2574.335496
	TS dissociative mechanism	no data					
	P dissociative mechanism	-2417.716021	-0.060689	373.687	240.668	23.074	-2417.258723
<b>2b</b>	S <i>trans</i>	-2496.371294	-0.052567	408.600	256.610	25.533	-2495.853889
	S <i>cis</i>	-2496.355843	-0.060856	408.997	249.042	25.148	-2495.843113
	TS interchange mechanism	-2653.484029	-0.049358	476.873	283.057	29.335	-2652.861117
	P interchange mechanism	-2653.515925	-0.050040	477.359	276.772	29.022	-2652.890433

	TS dissociative mechanism	no data					
	P dissociative mechanism	-2496.324666	-0.059237	408.122	256.816	25.361	-2495.815064
2c	S trans	-2571.329478	-0.049819	403.660	244.453	24.346	-2570.813315
	S cis	-2571.314616	-0.057331	403.969	245.913	24.628	-2570.805717
	TS interchange mechanism	-2728.443266	-0.046589	472.093	270.388	28.130	-2727.821105
	P interchange mechanism	-2728.474174	-0.047698	472.519	270.108	28.351	-2727.851958
	TS dissociative mechanism	no data					
	P dissociative mechanism	-2571.285802	-0.052919	403.287	258.402	25.293	-2570.778449

**Table S6.** Total energy values (E) and free energy values (G; as defined in the manuscript) for the initiation reaction following either the interchange or dissociative mechanism for **3a-c**. "S" stands for pre-catalyst, "TS" for transition state and "P" for product of the reaction (activated catalyst).

compound	structure	M06 Gas Phase, LACVP++ E (Hartrees)	solvation E in DCM (hartrees)	ZPE (kcal/mol)	S (cal/mol)	Thermal correction to enthalpy (kcal/mol)	G (Hartrees)
3a	S trans	-2388.270665	-0.058248	371.141	240.512	23.133	-2387.814815
	S cis	-2388.262774	-0.068542	371.470	233.676	22.810	-2387.813962
	TS interchange mechanism	-2545.395341	-0.052079	439.033	267.346	27.049	-2544.831633
	P interchange mechanism	-2545.404026	-0.055671	439.715	271.257	27.404	-2544.844115
	TS dissociative mechanism	-2388.248668	-0.059280	370.798	237.821	22.725	-2387.793769
	P dissociative mechanism	-2388.259648	-0.061823	371.288	241.250	23.116	-2387.807516
3b	S trans	-2466.865876	-0.056832	405.860	254.268	25.212	-2466.356502
	S cis	-2466.857539	-0.067169	406.340	247.169	24.863	-2466.354921
	TS interchange mechanism	-2623.998509	-0.050510	473.54	290.771	29.844	-2623.384912
	P interchange mechanism	-2623.999537	-0.054406	474.189	286.429	29.569	-2623.387177
	TS dissociative mechanism	-2466.843927	-0.058523	405.393	244.506	24.257	-2466.333874
	P dissociative mechanism	-2466.854621	-0.061271	406.018	262.619	25.767	-2466.352514
3c	S trans	-2541.856909	-0.056538	401.093	251.291	24.687	-2541.354260
	S cis	-2541.847907	-0.066123	401.228	253.000	24.994	-2541.354950
	TS interchange mechanism	-2698.981183	-0.050794	468.777	278.547	28.651	-2698.371555
	P interchange mechanism	-2698.990382	-0.054289	469.560	282.332	28.982	-2698.384272
	TS dissociative mechanism	-2541.834621	-0.057997	400.527	248.927	24.307	-2541.333816
	P dissociative mechanism	-2541.845785	-0.060031	401.209	251.710	24.674	-2541.346664

**Table S7.** Total energy values (E) and free energy values (G; as defined in the manuscript) for the initiation reaction following the dissociative mechanism for **3a-c** systems with the Na<sup>+</sup> counterion. "S" stands for pre-catalyst, "TS" for transition state and "P" for product of the reaction (activated catalyst).

compound	structure	M06 Gas Phase, LACVP++ E (Hartrees)	solvation E in DCM (hartrees)	ZPE (kcal/mol)	S (cal/mol)	Thermal correction to enthalpy (kcal/mol)	G (Hartrees)
3a Na <sup>+</sup>	S trans	-2550.154572	-0.028021	372.751	245.468	24.011	-2550.046220
	TS dissociative mechanism	-2550.131689	-0.030542	372.247	250.405	24.276	-2550.028762
	P dissociative mechanism	-2550.140608	-0.032342	372.866	251.715	24.569	-2550.037876

<b>3b</b> <b>Na<sup>+</sup></b>	S trans	-2628.735431	-0.027175	407.437	258.335	26.094	-2466.356502
	TS dissociative mechanism	-2628.713879	-0.028334	406.963	262.842	26.307	-2466.333874
	P dissociative mechanism	-2628.721537	-0.031665	407.494	265.574	26.687	-2466.352514
<b>3c</b> <b>Na<sup>+</sup></b>	S trans	-2703.702485	-0.027740	402.565	264.566	26.224	-2703.584679
	TS dissociative mechanism	-2703.680000	-0.028483	402.051	262.351	25.903	-2703.563256
	P dissociative mechanism	-2703.688243	-0.031623	402.642	263.430	26.210	-2703.572949

**Table S8.** Total energy values (E) and free energy values (G; as defined in the manuscript) for the initiation reaction following either the interchange or dissociative mechanism for **4a-c**. "S" stands for pre-catalyst, "TS" for transition state and "P" for product of the reaction (activated catalyst).

compound	structure	M06 Gas Phase, LACVP++ E (Hartrees)	solvation E in DCM (hartrees)	ZPE (kcal/mol)	S (cal/mol)	Thermal correction to enthalpy (kcal/mol)	G (Hartrees)
<b>4a</b>	S trans	-2492.595071	-0.019908	369.061	237.910	23.238	-2492.102794
	S cis	-2492.583903	-0.025014	369.295	234.141	23.029	-2492.094901
	TS interchange mechanism	-2649.709973	-0.015629	437.307	270.179	27.650	-2649.112953
	P interchange mechanism	-2649.738125	-0.018163	437.914	259.249	26.755	-2649.138906
	TS dissociative mechanism	-2492.547931	-0.018227	368.603	244.424	23.607	-2492.057207
	P dissociative mechanism	-2492.558719	-0.019241	368.603	244.424	23.607	-2492.069009
<b>4b</b>	S trans	-2531.895843	-0.018580	386.378	253.210	24.951	-2531.379176
	S cis	-2531.886402	-0.024012	386.768	238.998	24.015	-2531.369289
	TS interchange mechanism	-2689.012730	-0.014718	454.612	276.537	28.717	-2688.388540
	P interchange mechanism	-2689.040543	-0.016159	455.325	279.923	28.895	-2688.417983
	TS dissociative mechanism	-2531.854282	-0.017333	385.876	251.196	24.728	-2531.336568
	P dissociative mechanism	-2531.861393	-0.018514	385.876	251.196	24.728	-2531.344860
<b>5a</b>	S trans	-2492.594640	-0.019799	369.025	238.369	23.284	-2492.102455
	S cis	-2492.583607	-0.025946	369.424	239.758	23.542	-2492.097182
	TS interchange mechanism	-2649.707623	-0.016881	437.43	271.711	27.645	-2649.112394
	P interchange mechanism	-2649.738078	-0.017778	437.927	266.556	27.282	-2649.141084
	TS dissociative mechanism	-2492.546060	-0.019060	368.137	237.663	23.074	-2492.054551
	P dissociative mechanism	-2492.556804	-0.020538	368.506	238.497	23.109	-2492.066525
<b>5b</b>	S trans	-2531.896078	-0.019146	386.341	246.448	24.429	-2531.377657
	S cis	-2531.885036	-0.025616	386.729	247.835	24.663	-2531.372753
	TS interchange mechanism	-2689.009585	-0.016259	454.647	272.452	28.225	-2688.385724
	P interchange mechanism	-2689.038766	-0.016886	455.314	272.498	28.337	-2688.414312
	TS dissociative mechanism	-2531.849232	-0.018009	385.535	245.878	24.216	-2531.331028
	P dissociative mechanism	-2531.857711	-0.020082	385.862	252.542	24.774	-2531.343333

## Geometries in xyz format

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73
2a - S
Ru1 12.851083 5.719468 5.245438
C12 10.806763 4.889928 6.161490
C13 15.078137 6.536857 4.995014
O4 13.775323 3.867898 5.941797
N5 11.823244 8.457105 5.560670
N6 11.414452 7.923403 3.556086
N7 11.980010 7.464937 4.674039
C8 12.348471 8.347413 6.898191
C9 11.495848 7.883897 7.912498
C10 12.059957 7.734674 9.174344
H11 11.435574 7.358789 9.985241
C12 13.393691 8.064529 9.431398
C13 14.164500 8.613078 8.407183
H14 15.189388 8.921436 8.611779
C15 13.658972 8.791285 7.122484
C16 10.030338 7.660091 7.697969
H17 9.661892 6.854895 8.339940
H18 9.780455 7.384079 6.669327
H19 9.477222 8.572293 7.960013

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C20	13.965463	7.855891	10.799536	H27	14.217203	9.036520	5.035706
H21	15.043910	8.037133	10.821430	C28	11.499210	7.209139	2.356877
H22	13.782851	6.832401	11.147812	C29	10.523195	6.313175	1.901883
H23	13.496541	8.527523	11.528745	C30	10.740476	5.740215	0.651912
C24	14.455608	9.520065	6.084490	H31	10.009419	5.027675	0.268994
H25	15.526219	9.350401	6.227885	C32	11.862516	6.049248	-0.119464
H26	14.274067	10.600048	6.174266	C33	12.789751	6.967480	0.374847
H27	14.219365	9.212964	5.061689	H34	13.670432	7.211430	-0.219683
C28	11.396293	7.198441	2.312925	C35	12.631311	7.571040	1.617357
C29	10.272989	6.411476	2.029157	C36	9.308812	5.981507	2.713810
C30	10.273192	5.752179	0.804087	H37	8.770304	5.139171	2.271369
H31	9.417688	5.129344	0.542669	H38	8.607934	6.825962	2.754628
C32	11.334928	5.871091	-0.098098	H39	9.565644	5.715233	3.749095
C33	12.426592	6.671626	0.241099	C40	12.060862	5.398112	-1.453179
H34	13.255679	6.770825	-0.458891	H41	13.073830	5.557866	-1.835431
C35	12.487756	7.356416	1.452953	H42	11.357852	5.796939	-2.194571
C36	9.150066	6.260766	3.009249	H43	11.882127	4.317595	-1.395428
H37	8.357865	5.631399	2.595130	C44	13.645478	8.540070	2.144461
H38	8.700187	7.227722	3.270677	H45	14.342305	8.837065	1.355443
H39	9.494805	5.795669	3.945537	H46	14.235204	8.092410	2.957628
C40	11.295847	5.137563	-1.403576	H47	13.180707	9.453079	2.540580
H41	12.074235	5.485031	-2.088885	C48	12.790833	4.817503	3.800839
H42	10.325955	5.258388	-1.898322	H49	11.890840	4.220084	3.598925
H43	11.442379	4.061304	-1.250961	C50	16.384660	6.229291	5.053528
C44	13.679460	8.181414	1.830010	H51	16.991260	6.860832	4.386988
H45	14.358697	8.290648	0.980416	C52	16.154375	6.956597	6.350946
H46	14.242969	7.714013	2.652678	H53	15.720638	7.945788	6.185898
H47	13.396321	9.190116	2.159122	H54	17.117522	7.091600	6.855242
C48	12.829465	4.736395	3.680729	H55	15.500876	6.374475	7.011985
H49	12.411735	5.086337	2.732611	C56	17.022156	4.873394	5.259911
C50	14.111566	3.510830	7.328286	H57	17.214498	4.343501	4.322785
H51	15.104110	3.041746	7.274310	H58	16.377074	4.251552	5.889455
C52	14.209391	4.803165	8.099154	H59	17.983003	5.008238	5.768203
H53	14.923660	5.492473	7.636211	C60	15.059571	5.458262	3.174546
H54	14.547461	4.581738	9.117865	C61	16.105327	5.495069	2.260296
H55	13.226014	5.289444	8.174712	H62	17.017103	6.046760	2.468291
C56	13.065766	2.566467	7.874011	C63	15.986686	4.782838	1.069017
H57	12.979111	1.649100	7.283319	H64	16.814047	4.802510	0.363433
H58	12.088580	3.061488	7.882902	C65	14.844656	4.039120	0.773794
H59	13.330832	2.284734	8.899031	H66	14.784491	3.472096	-0.151301
C60	13.929797	2.973634	4.930525	C67	13.791177	4.033873	1.670507
C61	14.534379	1.730277	5.030425	H68	12.878820	3.476861	1.461478
H62	14.935188	1.361091	5.968654	C69	13.877281	4.753412	2.874395
C63	14.621461	0.948159	3.881127	C70	10.616508	9.281378	5.132150
H64	15.096749	-0.027210	3.951199	C71	10.462985	8.927309	3.827586
C65	14.116702	1.379219	2.652992	H72	10.184102	10.068318	5.733479
H66	14.199655	0.741950	1.777687	H73	9.866040	9.336169	3.025070
C67	13.515071	2.620391	2.564228	85			
H68	13.115354	2.988620	1.620552	2a - TS inter			
C69	13.415322	3.438035	3.702726	C80	14.506412	3.753134	7.417706
C70	11.166907	9.516698	5.019462	C81	13.873194	4.550541	8.319458
C71	10.903592	9.175542	3.730053	H82	14.268778	5.565465	8.430170
H72	10.957754	10.403225	5.600471	C83	12.801265	4.150375	9.271978
H73	10.413021	9.693062	2.917954	H84	13.224928	4.037681	10.279195
73				H85	12.020887	4.918251	9.328437
2a - S - cis				H86	12.319614	3.205479	9.002621
Ru1	12.923506	5.775585	5.360150	C87	14.274900	2.295634	7.220131
C12	10.788910	5.063726	6.019600	H88	13.283562	1.973594	7.554055
C13	13.846706	4.177021	6.758809	H89	14.404575	2.005416	6.170663
O4	15.070368	6.096388	4.386365	H90	15.020514	1.726174	7.791815
N5	11.522048	8.409385	5.652030	H91	15.346504	4.196647	6.879343
N6	11.286195	7.859497	3.623338	N1	11.505485	8.327553	5.616940
N7	11.935734	7.526439	4.740399	N2	11.282619	7.245661	3.802342
C8	12.128387	8.444920	6.960435	N3	11.947831	7.243932	4.966265
C9	11.434332	7.955441	8.071970	C4	12.080868	8.745723	6.875136
C10	12.116354	7.993824	9.288533	C5	11.403634	8.476295	8.070025
H11	11.614699	7.600910	10.172763	C6	12.051277	8.853867	9.246533
C12	13.396083	8.527066	9.410823	H7	11.557427	8.648844	10.196658
C13	14.001905	9.091438	8.282606	C8	13.278663	9.510438	9.240022
H14	14.977677	9.567902	8.379715	C9	13.854918	9.848525	8.012488
C15	13.385194	9.070572	7.040999	H10	14.786264	10.413925	7.996187
C16	10.016061	7.478532	8.040099	C11	13.274212	9.485063	6.806429
H17	9.940197	6.475251	8.471384	C12	10.010346	7.930764	8.144500
H18	9.597977	7.418894	7.032948	H13	9.937593	7.152236	8.911430
H19	9.392998	8.149722	8.644257	H14	9.665839	7.483537	7.210322
C20	14.108524	8.508177	10.726760	H15	9.320658	8.735823	8.430406
H21	14.832568	9.325171	10.806707	C16	13.965325	9.872894	10.519699
H22	14.660299	7.567444	10.848093	H17	14.410005	10.872366	10.466708
H23	13.408794	8.582619	11.565107	H18	14.781468	9.170631	10.728511
C24	13.997042	9.743024	5.847283	H19	13.279126	9.845994	11.371364
H25	14.933926	10.237657	6.120019	C20	13.882443	9.895521	5.500289
H26	13.330967	10.512665	5.433284	H21	14.621398	10.686224	5.657683



H22	13.132247	10.278226	4.795234	H30	13.444964	7.369717	11.247722
H23	14.401057	9.049098	5.033195	H31	12.562000	8.854715	11.600274
C24	11.538316	6.308232	2.736022	C32	14.703487	9.318970	6.215580
C25	10.683137	5.212119	2.572954	H33	15.687667	8.917273	6.471122
C26	10.985572	4.335505	1.533259	H34	14.768021	10.414694	6.251010
H27	10.347644	3.463297	1.385380	H35	14.497373	9.018103	5.184846
C28	12.070390	4.540768	0.681866	C36	11.852923	6.865483	2.371682
C29	12.848243	5.689922	0.847374	C37	10.724562	6.113096	2.029551
H30	13.675965	5.878452	0.163317	C38	10.827485	5.330215	0.881729
C31	12.602070	6.599369	1.869230	H39	9.967569	4.734534	0.576970
C32	9.512791	4.959315	3.467517	C40	11.990529	5.291541	0.115070
H33	8.802083	4.283489	2.982017	C41	13.084756	6.068633	0.504658
H34	8.975462	5.876457	3.735597	H42	13.996688	6.045375	-0.092476
H35	9.845183	4.509577	4.413469	C43	13.043036	6.882501	1.629510
C36	12.414917	3.533785	-0.370138	C44	9.465343	6.143653	2.841030
H37	12.921641	3.993757	-1.224536	H45	8.796894	5.333170	2.532867
H38	11.527831	3.007030	-0.735883	H46	8.919025	7.087034	2.704557
H39	13.096210	2.779019	0.048008	H47	9.658270	6.022703	3.917136
C40	13.464065	7.812001	2.055492	C48	12.084320	4.429085	-1.105416
H41	14.115629	7.959348	1.189896	H49	12.499371	4.982272	-1.955431
H42	14.110192	7.722805	2.941987	H50	11.107520	4.032970	-1.401632
H43	12.872241	8.727639	2.183701	H51	12.753913	3.578488	-0.918454
C44	10.572030	8.996858	4.888785	C52	14.217771	7.716734	2.035211
C45	10.432533	8.307722	3.724556	H53	14.987676	7.702233	1.258873
H46	9.828368	8.474101	2.844217	H54	14.668988	7.340271	2.966321
H47	10.114956	9.901615	5.263300	H55	13.940727	8.766044	2.206106
Ru48	12.938922	5.757982	5.913909	C56	12.465951	4.485600	4.214050
C149	10.787009	5.111993	6.699559	H57	11.393423	4.253968	4.207645
C150	15.124394	6.790389	6.023339	C58	10.408656	1.471871	2.298913
O51	11.942290	2.717398	5.042251	H59	11.073147	0.596680	2.237787
C52	13.579283	4.984692	4.343640	C60	9.336242	1.226899	3.334979
H53	14.127180	5.711068	3.728741	H61	9.775473	0.982134	4.306922
C54	11.083351	1.585068	5.350633	H62	8.689109	0.399628	3.025755
H55	11.736168	0.710466	5.496875	H63	8.717407	2.124412	3.454480
C56	10.367795	1.859515	6.650425	C64	9.831239	1.806696	0.939512
H57	11.069077	2.123872	7.448257	H65	10.605586	2.076377	0.211570
H58	9.823245	0.956430	6.948447	H66	9.134500	2.649895	1.032603
H59	9.654389	2.682589	6.548766	H67	9.273141	0.951874	0.542381
C60	10.104260	1.349126	4.216926	C68	12.468068	2.746327	2.493384
H61	10.597439	1.200770	3.250517	C69	13.132483	1.984627	1.527540
H62	9.427726	2.207543	4.131063	H70	12.602453	1.226018	0.959874
H63	9.495779	0.462701	4.426480	C71	14.482608	2.195649	1.288141
C64	12.928294	2.531076	4.158913	H72	14.981583	1.589486	0.534471
C65	13.225009	1.301963	3.550987	C73	15.204714	3.160942	1.992614
H66	12.649429	0.413506	3.782683	H74	16.261738	3.310461	1.792393
C67	14.269724	1.189832	2.644927	C75	14.564316	3.914409	2.953888
H68	14.477391	0.215598	2.207200	H76	15.106475	4.667555	3.522448
C69	15.040285	2.294397	2.281852	C77	13.190545	3.742374	3.236555
H70	15.853258	2.197554	1.568018	C78	11.456605	9.566849	4.681776
C71	14.740077	3.514116	2.850110	C79	11.294494	9.047066	3.434242
H72	15.318795	4.397387	2.582356	H80	11.241612	10.537510	5.104649
C73	13.714671	3.666267	3.814321	H81	10.909823	9.460161	2.512820
85				C82	12.545991	2.455751	6.471010
2a - P inter				H83	12.431094	2.006560	5.478513
C1	13.558875	3.556642	6.461044	H84	12.886697	1.663320	7.151109
C2	13.677561	4.529879	7.432386	H85	11.563860	2.799877	6.807519
H3	14.626386	5.072316	7.452086	H86	14.419464	3.428416	5.802297
C4	12.821197	4.673672	8.646841	73			
H5	12.594161	5.728495	8.853822	2a - P dis			
H6	11.875101	4.134647	8.574392	Ru9	12.938911	5.814787	5.437873
H7	13.383623	4.292562	9.511478	C110	11.171131	4.929742	6.739592
Ru9	12.850897	5.699299	5.622601	C111	15.185355	6.452040	5.057661
C110	10.554574	5.307728	6.348397	O12	11.034772	2.703425	2.792102
C111	15.182397	6.252150	5.235710	N13	11.869420	8.508996	5.475574
O12	11.177344	2.585707	2.801782	N14	11.662801	7.767007	3.487548
N13	12.002271	8.572217	5.430689	N15	12.102132	7.428897	4.713095
N14	11.756431	7.765548	3.494153	C16	12.260303	8.526583	6.861428
N15	12.184733	7.464067	4.716239	C17	11.296371	8.182112	7.821164
C16	12.339172	8.594655	6.833356	C18	11.712279	8.177762	9.145518
C17	11.297151	8.420243	7.758900	H19	10.995571	7.902496	9.918567
C18	11.660151	8.384480	9.099578	C20	13.016861	8.520357	9.511137
H19	10.881779	8.235876	9.847813	C21	13.914460	8.917740	8.521164
C20	12.987135	8.538458	9.511647	H22	14.919580	9.231094	8.802299
C21	13.966691	8.795652	8.553637	C23	13.559610	8.948692	7.175052
H22	14.993152	8.980466	8.869882	C24	9.870606	7.907064	7.454226
C23	13.667887	8.858261	7.193898	H25	9.379200	7.318856	8.233834
C24	9.856803	8.363992	7.351260	H26	9.776470	7.342710	6.520836
H25	9.270470	7.809226	8.088984	H27	9.313506	8.848034	7.346666
H26	9.706809	7.864826	6.389109	C28	13.436465	8.464436	10.946704
H27	9.440848	9.379681	7.293181	H29	14.290651	9.118878	11.144598
C28	13.340827	8.424811	10.961765	H30	13.733472	7.444332	11.219969
H29	14.288544	8.921563	11.189719	H31	12.618158	8.751916	11.614870

C32	14.503261	9.515101	6.158125	H31	9.446774	5.152992	0.589347
H33	15.534905	9.232623	6.386571	C32	11.380898	5.830997	-0.070058
H34	14.448263	10.611560	6.174464	C33	12.492714	6.611459	0.249986
H35	14.300160	9.177867	5.137193	H34	13.326432	6.668146	-0.449428
C36	11.799664	6.929527	2.323972	C35	12.569805	7.325324	1.444472
C37	10.709334	6.134452	1.950750	C36	9.215980	6.338032	3.032883
C38	10.862809	5.358007	0.806947	H37	8.368408	5.798423	2.601737
H39	10.037965	4.720097	0.491325	H38	8.851224	7.318510	3.367393
C40	12.044036	5.364709	0.065062	H39	9.540811	5.794339	3.933856
C41	13.084149	6.208686	0.458882	C40	11.323653	5.063734	-1.355895
H42	13.998943	6.241383	-0.132742	H41	12.119295	5.363534	-2.044052
C43	12.988191	7.019732	1.584304	H42	10.362518	5.207684	-1.861676
C44	9.437344	6.104786	2.743921	H43	11.427884	3.986697	-1.174574
H45	8.829069	5.241097	2.457131	C44	13.787658	8.118563	1.808159
H46	8.831511	7.004219	2.570323	H45	14.466059	8.201813	0.954828
H47	9.615324	6.038771	3.826330	H46	14.339588	7.639696	2.632537
C48	12.210502	4.465085	-1.119664	H47	13.539602	9.136852	2.136703
H49	12.748913	4.962041	-1.933501	C48	12.828544	4.726771	3.687677
H50	11.247133	4.117864	-1.506580	H49	12.415878	5.075524	2.737146
H51	12.797964	3.580091	-0.838497	C50	14.076146	3.484502	7.338975
C52	14.106144	7.932360	1.979166	H51	15.061048	2.998600	7.290804
H53	14.839045	8.014687	1.172044	C52	14.192209	4.773780	8.112312
H54	14.628492	7.556815	2.870549	H53	14.916222	5.453317	7.649340
H55	13.750361	8.945410	2.209017	H54	14.527490	4.546283	9.130690
C56	12.397236	4.668699	4.042751	H55	13.215709	5.274102	8.186865
H57	11.314305	4.634232	3.896594	C56	13.011407	2.557238	7.878173
C58	10.206566	1.609259	2.334181	H57	12.916043	1.640294	7.288045
H59	10.794897	0.683567	2.416070	H58	12.041990	3.067802	7.876808
C60	9.041546	1.553931	3.293210	H59	13.262830	2.273222	8.906053
H61	9.383354	1.389593	4.318931	C60	13.900912	2.950493	4.943632
H62	8.362484	0.741063	3.015950	C61	14.490012	1.699594	5.047175
H63	8.479635	2.495265	3.262571	H62	14.882080	1.326028	5.987458
C64	9.772697	1.848512	0.903000	C63	14.573329	0.915286	3.898995
H65	10.623800	2.010797	0.230912	H64	15.036737	-0.065619	3.972025
H66	9.119729	2.729603	0.853348	C65	14.079512	1.351806	2.668803
H67	9.202948	0.990567	0.530203	H66	14.159181	0.713675	1.793757
C68	12.352000	2.708241	2.580853	C67	13.492554	2.600195	2.577313
C69	13.015853	1.796500	1.756132	H68	13.102012	2.972927	1.631554
H70	12.465736	1.030105	1.219592	C69	13.397415	3.419562	3.714010
C71	14.395469	1.864195	1.621139	C70	11.313321	9.602355	4.975170
H72	14.892524	1.142524	0.976084	C71	11.050538	9.260111	3.674118
C73	15.152444	2.828190	2.292482	C72	11.064822	10.838965	5.748671
H74	16.230921	2.861809	2.170694	H73	10.602599	11.598824	5.114028
C75	14.514797	3.730372	3.114259	H74	10.396394	10.646632	6.595737
H76	15.079288	4.496724	3.640951	H75	11.999177	11.247515	6.149833
C77	13.109374	3.713000	3.275767	C76	10.423909	10.005188	2.558607
C78	11.277823	9.503240	4.457713	H77	10.138065	11.007254	2.887175
C79	11.142056	9.030665	3.791854	H78	11.111593	10.104203	1.710936
H80	11.018598	10.445255	5.218807	H79	9.525520	9.494850	2.192984
H81	10.737692	9.465044	2.588849	79			
2b - s				2b - s - cis			
Ru1	12.865425	5.718790	5.243837	Ru1	12.912657	5.771867	5.363952
C12	10.797098	4.947070	6.163949	C12	10.741847	5.143056	5.986832
C13	15.111568	6.491562	4.990465	C13	13.749659	4.171066	6.818083
O4	13.752712	3.848241	5.952954	O4	15.107032	6.008194	4.423310
N5	11.914842	8.506516	5.527381	N5	11.673754	8.499840	5.603451
N6	11.511571	7.976422	3.529203	N6	11.417630	7.959187	3.582061
N7	12.040857	7.502950	4.654629	N7	12.018051	7.577841	4.707042
C8	12.418173	8.372889	6.870123	C8	12.281756	8.485423	6.911183
C9	11.542006	7.919953	7.870645	C9	11.566080	8.024613	8.020171
C10	12.086136	7.732015	9.136285	C10	12.250510	8.010355	9.237180
H11	11.441076	7.358460	9.932171	H11	11.729478	7.633040	10.116940
C12	13.426501	8.012491	9.413561	C12	13.556947	8.470857	9.362395
C13	14.225740	8.551207	8.406701	C13	14.192857	9.009087	8.237263
H14	15.259652	8.817414	8.625549	H14	15.197442	9.421261	8.336921
C15	13.741709	8.765130	7.118780	C15	13.576374	9.031005	6.996191
C16	10.072896	7.728726	7.643418	C16	10.125496	7.621259	7.983070
H17	9.711820	6.836837	8.163437	H17	10.000097	6.609795	8.382516
H18	9.808407	7.606156	6.588543	H18	9.703625	7.612532	6.975010
H19	9.522594	8.590811	8.045059	H19	9.538977	8.303667	8.611605
C20	13.977451	7.756242	10.782537	C20	14.278595	8.403398	10.671933
H21	15.064945	7.871057	10.810705	H21	14.919656	9.278644	10.822620
H22	13.731428	6.742230	11.119365	H22	14.925793	7.517828	10.705547
H23	13.547624	8.447659	11.517329	H23	13.585252	8.333246	11.515208
C24	14.592073	9.465317	6.102903	C24	14.240756	9.643334	5.798218
H25	15.629693	9.126300	6.166626	H25	15.194256	10.102316	6.076407
H26	14.583847	10.546760	6.297998	H26	13.621580	10.428196	5.341813
H27	14.266565	9.296954	5.071862	H27	14.444495	8.899017	5.016083
C28	11.474019	7.221753	2.307112	C28	11.604546	7.271622	2.331782
C29	10.333594	6.453298	2.041684	C29	10.602142	6.399218	1.887457
C30	10.316419	5.763009	0.833880	C30	10.803970	5.797862	0.648093
				H31	10.050636	5.103256	0.275263

C32	11.938164	6.054199	-0.124931
C33	12.895547	6.945950	0.358316
H34	13.788838	7.145495	-0.234003
C35	12.752725	7.575152	1.590550
C36	9.380274	6.110207	2.703784
H37	8.782795	5.323605	2.235294
H38	8.734107	6.993022	2.800526
H39	9.636554	5.783907	3.721945
C40	12.118977	5.369917	-1.444833
H41	13.124318	5.526111	-1.848110
H42	11.399812	5.741292	-2.184857
H43	11.950993	4.289669	-1.354217
C44	13.806039	8.506109	2.110613
H45	14.517559	8.765588	1.321394
H46	14.373394	8.038871	2.928660
H47	13.383098	9.441803	2.501407
C48	12.782155	4.804235	3.813796
H49	11.870925	4.227149	3.602368
C50	16.417737	6.036963	5.111172
H51	17.079734	6.629442	4.461855
C52	16.227628	6.764409	6.415097
H53	15.879797	7.788165	6.258106
H54	17.191585	6.812963	6.933699
H55	15.518637	6.229623	7.058538
C56	16.952632	4.635681	5.307591
H57	17.122149	4.107309	4.365138
H58	16.254284	4.053374	5.917935
H59	17.912258	4.693542	5.832549
C60	15.078466	5.376060	3.207540
C61	16.132210	5.380679	2.301387
H62	17.059727	5.901588	2.519905
C63	16.002484	4.674807	1.107657
H64	16.836169	4.669311	0.409290
C65	14.840257	3.967637	0.802871
H66	14.769568	3.403185	-0.123126
C67	13.780153	3.994477	1.691851
H68	12.852919	3.465594	1.475087
C69	13.877446	4.709793	2.896881
C70	10.872899	9.470638	5.067020
C71	10.706461	9.120995	3.750263
C72	10.380157	10.617278	5.862195
H73	9.930750	11.370398	5.210398
H74	9.622034	10.298003	6.586943
H75	11.196864	11.086067	6.422827
C76	9.993579	9.785503	2.635844
H77	9.582267	10.742199	2.966885
H78	10.669940	9.972489	1.793661
H79	9.166089	9.171673	2.262156
91			
2b - TS inter			
C1	14.433875	3.726913	7.466427
C2	13.739593	4.464177	8.373489
H3	14.090631	5.488343	8.536462
C4	12.650759	3.985086	9.269115
H5	13.037632	3.861639	10.289801
H6	11.831768	4.712689	9.314130
H7	12.227771	3.026866	8.952298
C8	14.260660	2.270370	7.205393
H9	13.252180	1.915590	7.441366
H10	14.485192	2.018571	6.162060
H11	14.968281	1.698852	7.821562
H12	15.275607	4.221030	6.976758
N13	11.411093	8.327060	5.716638
N14	11.298652	7.337819	3.850576
N15	11.880534	7.268561	5.051590
C16	11.914494	8.666122	7.026789
C17	11.193712	8.297555	8.168033
C18	11.787180	8.585327	9.397566
H19	11.258605	8.297016	10.306706
C20	13.004329	9.253464	9.495271
C21	13.620591	9.702380	8.324069
H22	14.543881	10.277612	8.391515
C23	13.095591	9.427635	7.070086
C24	9.808213	7.726961	8.142774
H25	9.747903	6.811488	8.740524
H26	9.461865	7.466185	7.139565
H27	9.111894	8.453113	8.582703
C28	13.639116	9.510416	10.826681
H29	14.053585	10.522635	10.884831
H30	14.470644	8.814971	10.995567
H31	12.927962	9.382201	11.648116
C32	13.764128	9.937003	5.829882
H33	14.420119	10.778507	6.070193
H34	13.046508	10.278771	5.072273
H35	14.384265	9.149193	5.383937
C36	11.610719	6.425794	2.779741
C37	10.777830	5.323703	2.555681
C38	11.134033	4.472861	1.510897
H39	10.510430	3.596182	1.318167
C40	12.253725	4.706343	0.715138
C41	13.015441	5.855597	0.943245
H42	13.876770	6.060688	0.307016
C43	12.715637	6.739206	1.972907
C44	9.580221	5.027247	3.399818
H45	8.847671	4.442780	2.833894
H46	9.084058	5.929355	3.776756
H47	9.879592	4.457016	4.290439
C48	12.659854	3.724086	-0.338067
H49	13.191798	4.207267	-1.163910
H50	11.799946	3.184884	-0.747572
H51	13.339275	2.978019	0.097280
C52	13.572880	7.940811	2.239848
H53	14.254983	8.122850	1.404754
H54	14.186969	7.808764	3.144024
H55	12.982771	8.854157	2.392147
C56	10.548745	9.068793	4.957341
C57	10.479362	8.431352	3.744618
Ru58	12.854385	5.738011	5.983677
C159	10.688508	5.013943	6.654395
C160	15.011861	6.827535	6.203086
O61	11.985049	2.699108	4.979913
C62	13.582466	5.032524	4.423836
H63	14.134447	5.790365	3.851923
C64	11.132838	1.543028	5.195884
H65	11.791106	0.672589	5.342913
C66	10.344760	1.753881	6.465048
H67	10.998777	2.000393	7.307826
H68	9.803803	0.830433	6.700402
H69	9.622145	2.568003	6.357130
C70	10.223556	1.341328	3.999151
H71	10.775640	1.226237	3.060273
H72	9.551025	2.202112	3.900066
H73	9.606513	0.447472	4.141501
C74	13.019446	2.564405	4.142482
C75	13.383983	1.360637	3.521056
H76	12.821820	0.451018	3.696444
C77	14.484198	1.299936	2.678403
H78	14.745692	0.343441	2.230985
C79	15.243499	2.433342	2.391490
H80	16.101293	2.376815	1.727791
C81	14.873605	3.630422	2.967798
H82	15.441579	4.535952	2.757023
C83	13.787846	3.729936	3.869460
C84	9.912896	10.303484	5.468409
H85	9.369812	10.812672	4.668554
H86	9.204541	10.077841	6.273873
H87	10.663071	10.993019	5.871861
C88	9.748082	8.753490	2.498407
H89	9.194707	9.687633	2.618180
H90	10.436458	8.865764	1.652594
H91	9.034085	7.963837	2.237792
91			
2b - P inter			
C1	13.765289	3.575270	5.708537
C2	13.890628	4.419080	6.794692
H3	14.781655	5.052734	6.807520
C4	13.168173	4.284864	8.094780
H5	12.863880	5.264245	8.487201
H6	12.277252	3.657125	8.031509
H7	13.860855	3.845340	8.827483
Ru9	12.794828	5.725544	5.249890
C110	10.641072	5.052296	6.163982
C111	15.025041	6.525346	4.695026
O12	11.102741	2.771115	2.263388
N13	11.900656	8.590659	5.498974
N14	11.436859	8.033705	3.523240
N15	11.963625	7.573104	4.649449
C16	12.361709	8.414429	6.853821
C17	11.424875	8.008935	7.818617
C18	11.909100	7.781459	9.101546
H19	11.211862	7.451519	9.871938
C20	13.254919	7.965961	9.427342
C21	14.125292	8.448234	8.450728
H22	15.165119	8.648863	8.708904

C23	13.701054	8.707807	7.149212	H11	11.077935	7.681703	9.860610
C24	9.957183	7.904783	7.537617	C12	13.044799	8.436513	9.420835
H25	9.523968	7.051270	8.066199	C13	13.879987	8.944989	8.425672
H26	9.726767	7.764798	6.477087	H14	14.874000	9.304278	8.690984
H27	9.447221	8.810711	7.893103	C15	13.474046	9.026450	7.096911
C28	13.746791	7.640850	10.803588	C16	9.861320	7.760980	7.447868
H29	14.676460	8.167533	11.038886	H17	9.474227	7.002670	8.133869
H30	13.946841	6.564780	10.893363	H18	9.731756	7.370570	6.433605
H31	13.003060	7.893264	11.566632	H19	9.235575	8.658295	7.554481
C32	14.629277	9.369400	6.177624	C20	13.523764	8.319933	10.834228
H33	15.621357	8.910556	6.212699	H21	14.343127	9.014524	11.042854
H34	14.741671	10.428210	6.447445	H22	13.894604	7.306153	11.030308
H35	14.290283	9.307882	5.139058	H23	12.716687	8.511805	11.548755
C36	11.332893	7.228361	2.333913	C24	14.333840	9.710645	6.077984
C37	10.155556	6.498677	2.133413	H25	15.394070	9.541449	6.286586
C38	10.058941	5.789402	0.936958	H26	14.157071	10.794606	6.114281
H39	9.154733	5.211868	0.743426	H27	14.152976	9.366727	5.054740
C40	11.077934	5.806774	-0.014266	C28	11.680802	6.941885	2.298673
C41	12.229918	6.556131	0.240030	C29	10.636306	6.053233	2.013749
H42	13.032429	6.568409	-0.498389	C30	10.769687	5.275308	0.867740
C43	12.385306	7.289089	1.410189	H31	9.977584	4.570183	0.617535
C44	9.059083	6.467808	3.153328	C32	11.888027	5.367483	0.039248
H45	8.185648	5.936190	2.765550	C33	12.887896	6.289335	0.355759
H46	8.731773	7.476591	3.440828	H34	13.757722	6.378465	-0.295390
H47	9.382365	5.961622	4.076818	C35	12.808351	7.103876	1.480230
C48	10.957060	5.045599	-1.299136	C36	9.433461	5.926433	2.900831
H49	11.132170	5.696736	-2.163503	H37	8.847769	5.044056	2.623404
H50	9.967923	4.590369	-1.413412	H38	8.769351	6.797818	2.819963
H51	11.710364	4.246807	-1.344557	H39	9.702209	5.822223	3.961247
C52	13.625674	8.083839	1.681846	C40	12.033173	4.479365	-1.157395
H53	14.317268	8.019949	0.836743	H41	12.457731	5.017670	-2.011503
H54	14.151159	7.714852	2.576145	H42	11.073828	4.050638	-1.464896
H55	13.408728	9.147940	1.850566	H43	12.715002	3.647822	-0.929230
C56	12.350911	4.643917	3.756047	C44	13.892995	8.082846	1.805625
H57	11.320699	4.277335	3.851161	H45	14.566863	8.210947	0.953967
C58	10.425950	1.609677	1.737932	H46	14.491071	7.736291	2.661568
H59	11.185309	0.845439	1.511304	H47	13.498486	9.072950	2.070695
C60	9.534874	1.124660	2.857730	C48	12.534123	4.700151	3.984240
H61	10.122104	0.872892	3.746293	H49	11.460955	4.487216	3.957276
H62	8.979190	0.235150	2.543542	C50	10.637784	1.421018	2.330992
H63	8.814454	1.904311	3.131597	H51	11.350023	0.582925	2.307279
C64	9.643873	1.978441	0.494744	C52	9.587322	1.163985	3.385327
H65	10.284519	2.383719	-0.296515	H53	10.043675	1.002555	4.365938
H66	8.887333	2.733065	0.744276	H54	8.997654	0.279422	3.123231
H67	9.126554	1.098794	0.096632	H55	8.907470	2.021469	3.458190
C68	12.316608	3.128196	1.832107	C56	10.036132	1.658885	0.961347
C69	12.931471	2.565057	0.709130	H57	10.786933	1.955140	0.219241
H70	12.421221	1.809311	0.120061	H58	9.277287	2.449978	1.021750
C71	14.206387	2.968938	0.341024	H59	9.542318	0.749904	0.601235
H72	14.667047	2.516080	-0.534801	C60	12.619591	2.815266	2.426180
C73	14.902051	3.932891	1.072904	C61	13.315991	2.039139	1.495438
H74	15.902325	4.233533	0.774378	H62	12.830563	1.210601	0.989513
C75	14.311719	4.488032	2.188900	C63	14.645600	2.321706	1.216621
H76	14.840945	5.228933	2.784122	H64	15.170258	1.701914	0.492139
C77	13.013403	4.118069	2.605128	C65	15.318756	3.372425	1.845464
C78	11.341587	9.702798	4.933584	H66	16.360246	3.574068	1.613155
C79	11.036555	9.340963	3.644630	C67	14.649848	4.140366	2.772807
C82	12.867138	2.378524	5.664338	H68	15.152147	4.961768	3.279375
H83	12.718573	2.025100	4.638253	C69	13.290072	3.905074	3.083139
H84	13.334040	1.559766	6.228542	C70	11.121167	9.521530	4.730736
H85	11.885670	2.582131	6.103867	C71	10.973918	9.042195	3.455356
H86	14.561571	3.624290	4.964084	C72	10.358163	9.645018	2.251779
C86	11.164485	10.965220	5.685358	C73	10.714890	10.805926	5.348197
H87	10.824984	11.762601	5.019686	H74	11.223087	11.650171	4.869379
H88	10.424292	10.848708	6.485673	H75	9.635111	10.962381	5.250597
H89	12.106415	11.280698	6.147701	H76	10.966853	10.816310	6.412849
C89	10.415566	10.087543	2.526786	H77	9.915523	10.611871	2.505721
H90	10.182879	11.109191	2.837463	H78	11.098901	9.804664	1.459231
H91	11.084515	10.135301	1.659761	H79	9.571602	9.003377	1.838656
H92	9.485815	9.609542	2.197307	83			
79				2c - s			
2b - P dis				Ru1	12.882959	5.738961	5.239300
Ru1	13.019889	5.911898	5.350260	C12	10.817718	4.947573	6.138645
C12	11.284894	4.924266	6.646130	C13	15.141548	6.466944	5.002366
C13	15.192823	6.747264	4.871370	O	13.750571	3.856749	5.954172
O4	11.350184	2.598173	2.774617	N5	11.960817	8.483090	5.540861
N5	11.771845	8.537279	5.423870	N6	11.548824	7.944397	3.512511
N6	11.553097	7.797353	3.446432	N7	12.081205	7.485107	4.649915
N7	12.038096	7.477528	4.652219	C10	12.472006	8.355251	6.878057
C8	12.193816	8.535670	6.800393	C11	11.595483	7.929330	7.891079
C9	11.286236	8.089297	7.772221	C12	12.140771	7.770327	9.160090
C10	11.749387	8.040667	9.081076	H13	11.496345	7.420247	9.967015

C14	13.481065	8.061344	9.429818	C15	14.268897	9.109634	8.250292
C15	14.277618	8.583593	8.411649	H16	15.265951	9.541126	8.343705
H16	15.307767	8.866729	8.626912	C17	13.656125	9.094668	7.007878
C17	13.790955	8.768046	7.120065	C18	10.214559	7.681297	8.020008
C18	10.124376	7.758768	7.664182	H19	10.104624	6.637821	8.333089
H19	9.717131	6.978810	8.314198	H20	9.758370	7.764423	7.031000
H20	9.875378	7.480846	6.635824	H21	9.647605	8.304184	8.722287
H21	9.604649	8.696724	7.904557	C22	14.344046	8.581774	10.703710
C22	14.032605	7.839423	10.804590	H23	14.967526	9.473298	10.832313
H23	15.110591	8.020906	10.844892	H24	15.007354	7.710195	10.771622
H24	13.846610	6.811479	11.138507	H25	13.644000	8.525794	11.542616
H25	13.551728	8.501322	11.534930	C26	14.305456	9.713846	5.805728
C26	14.618690	9.474050	6.090423	H27	15.276884	10.143837	6.067940
H27	15.682017	9.263114	6.235284	H28	13.690518	10.524207	5.389693
H28	14.476402	10.559564	6.188072	H29	14.469143	8.986529	4.999127
H29	14.371420	9.187211	5.064251	C30	11.720688	7.317706	2.311417
C30	11.514771	7.210372	2.280846	C31	10.690495	6.501214	1.823463
C31	10.363249	6.467478	1.989306	C32	10.896340	5.911643	0.578920
C32	10.342416	5.805483	0.766008	H33	10.121562	5.260081	0.173912
H33	9.464240	5.216216	0.501609	C34	12.060901	6.129499	-0.159808
C34	11.410928	5.882884	-0.132565	C35	13.041454	6.975219	0.359814
C35	12.528566	6.646697	0.207234	H36	13.953808	7.151047	-0.210674
H36	13.361266	6.717869	-0.492219	C37	12.893653	7.592477	1.596755
C37	12.608899	7.332209	1.417807	C38	9.430433	6.270968	2.598964
C38	9.230353	6.368262	2.964493	H39	8.812491	5.510900	2.113509
H39	8.403918	5.790381	2.541975	H40	8.829373	7.187431	2.667667
H40	8.839312	7.357829	3.236555	H41	9.636148	5.940191	3.626805
H41	9.545761	5.874943	3.896496	C42	12.246659	5.461592	-1.487179
C42	11.348057	5.149813	-1.437728	H43	13.279750	5.541546	-1.839617
H43	12.150338	5.456487	-2.115358	H44	11.598719	5.911408	-2.249235
H44	10.390611	5.320757	-1.942433	H45	11.983555	4.398200	-1.434555
H45	11.436473	4.066941	-1.284476	C46	13.960721	8.487549	2.148514
C46	13.820124	8.129001	1.794114	H47	14.707616	8.716844	1.382988
H47	14.514989	8.199855	0.952910	H48	14.482812	8.009024	2.989937
H48	14.357638	7.665638	2.636017	H49	13.551976	9.439530	2.513710
H49	13.558231	9.151944	2.096412	C50	12.766070	4.859255	3.774425
C50	12.847883	4.743483	3.680075	H51	11.827108	4.338655	3.541602
H51	12.446646	5.098528	2.727739	C52	16.427311	5.992415	5.137523
C52	14.070041	3.492318	7.343222	H53	17.099001	6.567471	4.482276
H53	15.051459	2.999545	7.295220	C54	16.206806	6.757561	6.414564
C54	14.193808	4.781764	8.114985	H55	15.852429	7.771945	6.217754
H55	14.926963	5.454213	7.656607	H56	17.158287	6.831249	6.952612
H56	14.520975	4.551927	9.135459	H57	15.488673	6.237559	7.060590
H57	13.221904	5.291419	8.185119	C58	16.958447	4.598123	5.385705
C58	12.998671	2.573130	7.882697	H59	17.137881	4.037527	4.463879
H59	12.891019	1.659366	7.289850	H60	16.252591	4.036195	6.006201
H60	12.034182	3.092493	7.889250	H61	17.911869	4.673235	5.919771
H61	13.252707	2.282663	8.908151	C62	15.103919	5.297289	3.225921
C62	13.890887	2.957963	4.946170	C63	16.180359	5.231025	2.349828
C63	14.463168	1.699645	5.051775	H64	17.129858	5.701268	2.586843
H64	14.847932	1.321480	5.993210	C65	16.039784	4.521685	1.159342
C65	14.538538	0.914125	3.903954	H66	16.889735	4.461231	0.483531
H66	14.988651	-0.072869	3.978968	C67	14.846594	3.880969	0.827238
C67	14.053713	1.354904	2.670913	H68	14.767959	3.314408	-0.096659
H68	14.127085	0.713768	1.797588	C69	13.766475	3.977620	1.685857
C69	13.484473	2.610432	2.575460	H70	12.815583	3.503061	1.447555
H70	13.100844	2.988344	1.628496	C71	13.874352	4.697357	2.888246
C71	13.398136	3.431941	3.712693	C72	10.973932	9.503116	5.076556
C72	11.354293	9.579005	4.985051	C73	10.819631	9.158582	3.735976
C73	11.086161	9.230401	3.664889	C74	10.100132	9.955430	2.845500
C74	10.471449	10.107619	2.772599	C75	9.540373	11.100626	3.382411
C75	10.140822	11.348025	3.286194	C76	9.694843	11.447245	4.742356
C76	10.412287	11.701656	4.625773	C77	10.418469	10.660795	5.619745
C77	11.025341	10.829389	5.506020	H80	9.992325	9.683963	1.798791
H80	10.270027	9.822305	1.743622	H81	8.964818	11.758743	2.737434
H81	9.657595	12.076078	2.640699	H82	9.233187	12.360863	5.105684
H82	10.129954	12.691812	4.972363	H83	10.552528	10.915608	6.667507
H83	11.242698	11.088873	6.538724	91			
83				2c	- TS inter		
2c	- S - cis			C1	14.879546	4.125292	7.340602
Ru1	12.922865	5.803758	5.342350	C2	14.192590	4.865751	8.251439
C12	10.730685	5.239524	5.941052	H3	14.422073	5.937972	8.267815
C13	13.690049	4.130633	6.751370	C4	13.261725	4.379606	9.306064
O	15.128868	5.943873	4.430714	H5	13.674886	4.598674	10.299469
N5	11.760648	8.520711	5.623493	H6	12.292947	4.891836	9.234151
N6	11.523690	7.988122	3.565236	H7	13.077810	3.303915	9.244468
N7	12.099765	7.603834	4.710087	C8	14.902988	2.642972	7.208691
C10	12.371918	8.522978	6.927101	H9	14.109866	2.139935	7.767205
C11	11.653661	8.090847	8.046894	H10	14.828957	2.339119	6.156772
C12	12.331721	8.119814	9.267618	H11	15.867332	2.262644	7.571553
H13	11.806265	7.770880	10.156464	H12	15.586394	4.669878	6.712184
C14	13.632745	8.596021	9.386780	N13	11.442725	8.272831	5.624319

N14	11.314114	7.275975	3.726420	H3	14.587330	5.177352	7.484787
N15	11.877790	7.203435	4.939603	C4	12.811660	4.618020	8.658555
C16	11.940616	8.560371	6.946220	H5	12.497323	5.646688	8.879857
C17	11.164205	8.224465	8.065424	H6	11.913792	4.003858	8.572389
C18	11.745253	8.435244	9.314307	H7	13.399962	4.268923	9.519626
H19	11.173909	8.168404	10.203708	Ru9	12.822525	5.708677	5.623419
C20	13.014584	8.993757	9.455730	C110	10.566792	5.191092	6.372538
C21	13.688465	9.429418	8.312660	C111	15.143274	6.326585	5.241118
H22	14.647163	9.937468	8.415205	O12	11.297379	2.513258	2.792614
C23	13.162571	9.250210	7.039718	N13	12.128268	8.573579	5.427697
C24	9.735701	7.782309	7.980677	N14	11.794497	7.760265	3.480476
H25	9.538282	6.962730	8.678527	N15	12.184282	7.446602	4.715656
H26	9.445818	7.435379	6.986558	C16	12.379207	8.546819	6.844106
H27	9.084291	8.621154	8.261882	C17	11.275568	8.336870	7.690499
C28	13.641471	9.143954	10.807082	C18	11.537022	8.268744	9.052770
H29	14.267054	10.040761	10.863381	H19	10.707514	8.091570	9.737358
H30	14.289593	8.285506	11.026470	C20	12.827328	8.435585	9.565446
H31	12.889221	9.196395	11.600162	C21	13.868673	8.737603	8.689209
C32	13.816407	9.885761	5.851418	H22	14.864635	8.934522	9.086023
H33	14.893185	9.989189	6.008746	C23	13.669883	8.829666	7.312073
H34	13.398850	10.891468	5.701911	C24	9.870234	8.295294	7.174089
H35	13.681176	9.319568	4.925934	H25	9.221707	7.749271	7.864458
C36	11.622853	6.400139	2.628972	H26	9.785742	7.799762	6.202021
C37	10.798109	5.291958	2.391286	H27	9.476468	9.317066	7.079956
C38	11.081593	4.530561	1.261938	C28	13.073299	8.292350	11.035303
H39	10.468781	3.652865	1.053376	H29	13.989004	8.803438	11.347150
C40	12.120645	4.861230	0.389906	H30	13.179522	7.232801	11.303787
C41	12.900841	5.985803	0.663238	H31	12.238207	8.688948	11.622458
H42	13.709662	6.254465	-0.016468	C32	14.767234	9.329032	6.424248
C43	12.673652	6.781320	1.782696	H33	15.729065	8.889475	6.704299
C44	9.678894	4.932054	3.315459	H34	14.851928	10.418381	6.537216
H45	9.102812	4.092230	2.916154	H35	14.607308	9.101886	5.366756
H46	8.987677	5.771790	3.467058	C36	11.767911	6.827191	2.388744
H47	10.058184	4.654024	4.309783	C37	10.575822	6.139574	2.131141
C48	12.402769	4.003052	-0.803271	C38	10.560798	5.319357	1.004115
H49	13.085575	4.490078	-1.505772	H39	9.647955	4.772182	0.768120
H50	11.482786	3.747157	-1.340134	C40	11.669590	5.195234	0.168217
H51	12.862378	3.057145	-0.487526	C41	12.828992	5.916996	0.467001
C52	13.540859	7.965283	2.085386	H42	13.697987	5.825563	-0.185674
H53	14.234152	8.157824	1.262090	C43	12.904885	6.756955	1.570487
H54	14.141133	7.801321	2.994801	C44	9.375540	6.281119	3.015260
H55	12.952458	8.879216	2.242504	H45	8.527213	5.725054	2.606236
Ru56	12.933613	5.795928	5.870852	H46	9.067309	7.331046	3.114826
C157	10.841957	5.049747	6.767318	H47	9.571280	5.902571	4.030447
C158	15.053312	6.939675	5.570089	C48	11.636694	4.316380	-1.044825
O59	12.139710	2.582985	5.658882	H49	11.936525	4.869385	-1.942685
C60	13.441679	4.830413	4.347180	H50	10.640069	3.899176	-1.221803
H61	13.993772	5.464739	3.641412	H51	12.343966	3.482401	-0.935057
C62	11.251632	1.566999	6.202085	C52	14.140399	7.546356	1.877097
H63	11.706650	0.585059	6.008041	H53	14.936228	7.308269	1.165160
C64	11.174642	1.755793	7.697622	H54	14.519772	7.333337	2.887811
H65	12.153786	1.620197	8.168152	H55	13.954980	8.627663	1.815639
H66	10.497408	1.002566	8.115412	C56	12.488755	4.468666	4.219585
H67	10.796666	2.751113	7.948134	H57	11.442777	4.139832	4.258089
C68	9.898712	1.682852	5.531433	C58	10.612250	1.330095	2.327082
H69	9.970148	1.581985	4.441934	H59	11.343710	0.508668	2.281720
H70	9.459388	2.660447	5.764008	C60	9.572413	1.030873	3.381692
H71	9.225014	0.902098	5.900900	H61	10.038603	0.855861	4.356250
C72	12.699139	2.385039	4.469379	H62	8.995724	0.141977	3.105981
C73	12.648376	1.170029	3.768552	H63	8.880779	1.876194	3.478385
H74	12.077966	0.332818	4.153348	C64	9.998330	1.582318	0.966216
C75	13.343810	1.003230	2.582083	H65	10.745285	1.866532	0.216550
H76	13.297258	0.038040	2.081978	H66	9.259169	2.389934	1.037986
C77	14.101351	2.037279	2.030180	H67	9.483710	0.683260	0.610270
H78	14.665377	1.888447	1.113433	C68	12.569562	2.759264	2.471490
C79	14.107540	3.254716	2.672411	C69	13.268380	2.045632	1.491996
H80	14.659677	4.090160	2.244405	H70	12.780441	1.254163	0.931675
C81	13.407565	3.480988	3.887223	C71	14.596358	2.346455	1.230832
C82	10.615060	9.046947	4.852263	H72	15.121872	1.777691	0.466216
C83	10.529352	8.401606	3.621856	C73	15.264330	3.355573	1.928481
C84	9.784043	8.916673	2.562370	H74	16.306136	3.575352	1.713306
C85	9.128500	10.107618	2.815107	C75	14.591551	4.060274	2.903251
C86	9.215547	10.761514	4.062673	H76	15.095384	4.840666	3.469286
C87	9.959994	10.249981	5.109227	C77	13.236964	3.796690	3.210630
H88	9.731298	8.406536	1.604361	C82	12.713994	2.430260	6.447057
H89	8.529794	10.558854	2.028764	H83	12.657149	1.973484	5.453058
H90	8.682287	11.698004	4.200271	H84	13.087575	1.663037	7.138577
H91	10.041763	10.744759	6.073311	H85	11.702170	2.708122	6.757078
91				H86	14.522990	3.543087	5.810274
2c - P inter				C87	11.485421	9.098646	3.389601
C1	13.649216	3.598241	6.462382	C88	11.702967	9.627075	4.659722
C2	13.683554	4.563181	7.448107	C89	11.488493	10.972280	4.954401

C90	11.045274	11.751152	3.901932	C74	10.392488	11.594899	4.085206
C91	10.825585	11.216904	2.613921	C75	10.931782	10.824171	5.100740
C92	11.039073	9.881549	2.325512	H76	10.494963	9.420794	1.419454
H95	11.660578	11.369441	5.951196	H77	9.809983	11.751153	2.016765
H96	10.858584	12.808613	4.067498	H78	10.083580	12.613870	4.301062
H97	10.477448	11.879376	1.826233	H79	11.065171	11.193225	6.114308
H98	10.874818	9.457209	1.338617	73			
83				3a	-	S	
2c	-	P	dis	Ru1	12.788463	5.530150	5.412786
Ru1	12.871147	5.818668	5.431851	C12	10.659412	4.637883	6.099041
C12	11.166773	4.851872	6.743554	C13	14.906802	6.460803	5.988545
C13	15.120948	6.449674	5.100038	O4	13.781309	3.240616	5.888247
O4	11.026028	2.666533	2.798581	N5	11.748174	8.447469	5.720965
N5	11.870429	8.510393	5.469557	N6	11.293802	7.708524	3.611636
N6	11.625207	7.747347	3.466805	B7	11.948112	7.274927	4.853726
N7	12.064413	7.422980	4.700820	C8	12.328206	8.760293	6.979169
C8	12.268005	8.513354	6.849810	C9	11.698890	8.359874	8.166433
C9	11.315112	8.144326	7.812900	C10	12.312057	8.662048	9.381798
C10	11.731275	8.142477	9.137856	H11	11.829576	8.343982	10.309177
H11	11.021256	7.847492	9.909922	C12	13.513198	9.365100	9.443457
C12	13.025669	8.519034	9.504685	C13	14.095205	9.784942	8.251145
C13	13.911231	8.946392	8.515629	H14	15.036189	10.338520	8.279862
H14	14.906787	9.287484	8.798644	C15	13.522376	9.495418	7.014269
C15	13.554926	8.972343	7.170215	C16	10.379017	7.651746	8.130277
C16	9.892850	7.851467	7.447025	H17	9.964019	7.551919	9.140443
H17	9.407047	7.259072	8.226989	H18	10.458759	6.650569	7.685312
H18	9.803054	7.289311	6.512186	H19	9.657514	8.199637	7.510089
H19	9.328778	8.787986	7.337303	C20	14.142764	9.687791	10.768017
C20	13.447445	8.470943	10.940119	H21	15.183148	10.011751	10.648497
H21	14.278887	9.153438	11.140830	H22	14.137603	8.818663	11.437975
H22	13.779614	7.460604	11.209338	H23	13.606009	10.493794	11.287181
H23	12.620098	8.727470	11.609899	C24	14.198578	9.912297	5.744963
C24	14.477400	9.568690	6.151487	H25	15.042588	10.580817	5.951644
H25	15.522235	9.401282	6.428689	H26	13.509106	10.417432	5.056523
H26	14.318561	10.654365	6.096323	H27	14.581951	9.020075	5.230351
H27	14.339328	9.154269	5.148110	C28	11.316923	7.134452	2.317953
C28	11.773556	6.906327	2.314141	C29	10.294648	6.265859	1.913064
C29	10.686106	6.114911	1.923046	C30	10.368173	5.698997	0.641792
C30	10.849055	5.341828	0.778286	H31	9.579933	5.013506	0.322642
H31	10.024439	4.710675	0.448665	C32	11.424085	5.974742	-0.226028
C32	12.036772	5.351269	0.046535	C33	12.418699	6.853953	0.196207
C33	13.073282	6.194547	0.451587	H34	13.254301	7.079566	-0.470089
H34	13.992149	6.231575	-0.133811	C35	12.383663	7.439953	1.460875
C35	12.965551	7.001395	1.578782	C36	9.173964	5.941347	2.851011
C36	9.404547	6.094311	2.700762	H37	8.426427	5.303228	2.365616
H37	8.770378	5.263705	2.374663	H38	8.678468	6.853546	3.207213
H38	8.833692	7.021888	2.559347	H39	9.549457	5.427791	3.748148
H39	9.569526	5.982751	3.781541	C40	11.502046	5.310822	-1.570712
C40	12.212489	4.459371	-1.142626	H41	12.173672	5.852051	-2.247494
H41	12.755284	4.962789	-1.949728	H42	10.516689	5.249432	-2.049568
H42	11.252199	4.112891	-1.537968	H43	11.881499	4.282858	-1.488763
H43	12.800131	3.573571	-0.864136	C44	13.497647	8.321418	1.939212
C44	14.074211	7.921433	1.983632	H45	14.220510	8.516406	1.138658
H45	14.825241	7.992563	1.191960	H46	14.028505	7.847792	2.778245
H46	14.577691	7.562700	2.892518	H47	13.123219	9.281420	2.317707
H47	13.708836	8.936728	2.188106	C48	13.069475	4.810327	3.761178
C48	12.351317	4.665719	4.027666	H49	12.857297	5.335804	2.820037
H49	11.268525	4.611256	3.885910	C50	13.814803	2.485600	7.102476
C50	10.209098	1.574533	2.316772	H51	14.740593	1.883436	7.111359
H51	10.805207	0.652391	2.383012	C52	13.874638	3.508772	8.214848
C52	9.042127	1.493127	3.271871	H53	14.713002	4.196669	8.063320
H53	9.382365	1.310516	4.295071	H54	13.980218	3.005344	9.183695
H54	8.368101	0.682355	2.976746	H55	12.950002	4.100951	8.222044
H55	8.476005	2.432367	3.258390	C56	12.587541	1.599846	7.201520
C56	9.775611	1.837901	0.889822	H57	12.547348	0.860052	6.394300
H57	10.625598	2.017551	0.220789	H58	11.692768	2.232111	7.132635
H58	9.117855	2.716135	0.857266	H59	12.581969	1.067472	8.160792
H59	9.210862	0.983533	0.501404	C60	13.958733	2.658657	4.683182
C60	12.338505	2.704328	2.569489	C61	14.463562	1.375969	4.491372
C61	13.016263	1.809156	1.737582	H62	14.721487	0.751869	5.343368
H62	12.479826	1.030058	1.205399	C63	14.644890	0.890698	3.197336
C63	14.392874	1.908396	1.593246	H64	15.042314	-0.113671	3.058781
H64	14.901595	1.198703	0.943777	C65	14.322887	1.674095	2.095344
C65	15.133644	2.888054	2.261173	H66	14.463598	1.289359	1.087089
H66	16.210221	2.946053	2.131322	C67	13.813295	2.951718	2.294201
C67	14.482454	3.774273	3.088803	H68	13.544800	3.582823	1.445420
H68	15.033030	4.552076	3.613154	C69	13.617380	3.474815	3.577919
C69	13.078630	3.725448	3.259394	C70	11.055004	9.438838	5.019724
C70	11.303175	9.529731	4.745721	C71	10.789095	9.006027	3.771495
C71	11.142831	9.038299	3.452879	H72	10.794177	10.379102	5.494205
C72	10.605808	9.812168	2.427110	H73	10.255516	9.498748	2.965619
C73	10.234281	11.099619	2.775522	73			

3a - S - cis			
Ru1	12.979466	5.541920	5.476794
C12	10.763530	4.697325	5.704846
C13	13.577856	4.671461	7.723879
O	15.218819	6.055778	4.899682
N5	11.773310	8.402378	5.660867
N6	11.476454	7.676569	3.516233
B7	12.070383	7.262650	4.786091
C10	12.346165	8.758605	6.911316
C11	11.827501	8.251707	8.111329
C12	12.418928	8.653991	9.309254
H13	12.021379	8.257750	10.245751
C14	13.489733	9.542024	9.346588
C15	13.974466	10.044675	8.140882
H16	14.817274	10.740136	8.147738
C17	13.423460	9.661043	6.920394
C18	10.669284	7.306469	8.117874
H19	10.196819	7.279864	9.106588
H20	10.989802	6.286307	7.863273
H21	9.920754	7.582289	7.366711
C22	14.123404	9.923966	10.652778
H23	14.614187	10.902964	10.592925
H24	14.887075	9.194390	10.953757
H25	13.383757	9.964330	11.461712
C26	13.995707	10.170786	5.630385
H27	14.930667	10.717200	5.804976
H28	13.301680	10.834650	5.098410
H29	14.200077	9.336874	4.942333
C30	11.571236	7.117639	2.215780
C31	10.546016	6.300488	1.721675
C32	10.667709	5.786896	0.428878
H33	9.877475	5.138946	0.043801
C34	11.767084	6.073841	-0.375769
C35	12.759088	6.910517	0.130780
H36	13.635056	7.136842	-0.481812
C37	12.680600	7.436926	1.416563
C38	9.357432	5.983112	2.573504
H39	8.644018	5.351386	2.031706
H40	8.840423	6.898521	2.889840
H41	9.662764	5.469419	3.497738
C42	11.916649	5.465594	-1.739929
H43	12.246052	6.205977	-2.480112
H44	10.975924	5.028698	-2.093946
H45	12.670531	4.665230	-1.735330
C46	13.778416	8.302721	1.954835
H47	14.581425	8.422959	1.218018
H48	14.212184	7.860140	2.861947
H49	13.408212	9.297107	2.240312
C50	13.081186	4.913599	3.760029
H51	12.270452	4.350823	3.268345
C52	16.346050	6.292317	5.783181
H53	17.108167	6.824950	5.193176
C54	15.880726	7.204701	6.889908
H55	15.496717	8.146213	6.485682
H56	16.730618	7.432874	7.546093
H57	15.093943	6.723816	7.484923
C58	16.875087	4.965192	6.283022
H59	17.180384	4.316225	5.453684
H60	16.086582	4.465892	6.861062
H61	17.744864	5.129150	6.931161
C62	15.456122	5.566755	3.642505
C63	16.674390	5.649216	2.975741
H64	17.551827	6.073731	3.454510
C65	16.771141	5.181693	1.665542
H66	17.726341	5.256513	1.148428
C67	15.669527	4.624937	1.025405
H68	15.751447	4.267146	0.000386
C69	14.465263	4.521288	1.709281
H70	13.584917	4.091455	1.230049
C71	14.330736	4.985553	3.021935
C72	11.063493	9.366129	4.934580
C73	10.886910	8.938483	3.669431
H72	10.360056	9.411021	2.847391
H73	10.724507	10.281714	5.407031
85			
3a - TS inter			
C80	14.307718	3.575891	7.635724
C81	14.384088	4.888762	7.905282
H82	15.183249	5.450907	7.421709
C83	13.544623	5.671105	8.867740
H84	14.090889	5.850461	9.806067
H85	13.304756	6.664301	8.458120
H86	12.599101	5.172742	9.106306
C87	13.335557	2.592422	8.198300
H88	12.478279	3.084290	8.669697
H89	12.939856	1.948886	7.401023
H90	13.815320	1.936891	8.940881
H91	15.036503	3.172141	6.927600
N1	11.175727	8.205829	5.307133
N2	10.730584	6.822342	3.543287
B3	11.578283	6.905794	4.744182
C4	11.753077	9.006247	6.332465
C5	11.301852	8.899824	7.654610
C6	11.884159	9.714290	8.627900
H7	11.537950	9.629495	9.660376
C8	12.876258	10.638015	8.314428
C9	13.268496	10.759942	6.983518
H10	14.029873	11.495720	6.715314
C11	12.722138	9.961543	5.982203
C12	10.185159	7.968009	8.010632
H13	9.926267	8.058678	9.072199
H14	10.439344	6.921840	7.796528
H15	9.288262	8.186674	7.415591
C16	13.516474	11.478619	9.380892
H17	13.791693	12.470527	9.001078
H18	14.437139	11.013558	9.758027
H19	12.849179	11.618162	10.239972
C20	13.167472	10.111950	4.560241
H21	13.832998	10.976075	4.448700
H22	12.316772	10.232792	3.876856
H23	13.713185	9.210437	4.250129
C24	10.776736	5.962957	2.416735
C25	10.013278	4.788916	2.385706
C26	10.088668	3.974183	1.256765
H27	9.494460	3.057397	1.226636
C28	10.894261	4.299117	0.166463
C29	11.626816	5.482615	0.214490
H30	12.263720	5.754137	-0.630369
C31	11.582889	6.323002	1.326197
C32	9.146748	4.431444	3.550989
H33	8.592942	3.503188	3.359963
H34	8.424676	5.229404	3.768459
H35	9.747825	4.315090	4.464701
C36	10.989787	3.380170	-1.017120
H37	11.329420	3.912969	-1.913233
H38	10.022914	2.915155	-1.246303
H39	11.702553	2.564447	-0.834655
C40	12.431716	7.557045	1.397301
H41	12.991274	7.706706	0.466740
H42	13.150779	7.485160	2.226989
H43	11.831298	8.454729	1.594939
C44	10.191103	8.781156	4.497558
C45	9.930893	7.970642	3.454732
H46	9.218911	8.089979	2.645062
H47	9.745299	9.735661	4.757865
Ru48	12.842177	5.585224	5.612926
C149	10.922322	4.676217	6.759025
C150	14.712562	7.115665	5.470476
O51	12.266042	2.373789	5.018813
C52	13.192632	4.721228	4.067096
H53	12.928392	5.070721	3.058675
C54	11.503410	1.169545	5.021509
H55	12.054286	0.385012	5.571536
C56	10.221539	1.459593	5.767853
H57	10.431759	1.845171	6.770125
H58	9.619040	0.545444	5.841534
H59	9.642369	2.227271	5.242508
C60	11.246162	0.725470	3.592229
H61	12.179521	0.501360	3.063071
H62	10.737319	1.537655	3.054458
H63	10.609326	-0.167570	3.567599
C64	13.559226	2.324098	4.612601
C65	14.377488	1.196054	4.677044
H66	13.987503	0.245954	5.034727
C67	15.712899	1.289454	4.290771
H68	16.346268	0.405593	4.352931
C69	16.235386	2.493448	3.834356
H70	17.280978	2.563131	3.540439
C71	15.409404	3.610521	3.753517
H72	15.796819	4.569241	3.409972
C73	14.069285	3.542916	4.135165
85			
3a - P inter			
C1	13.596341	3.086333	6.786701



C2	13.646541	4.039564	7.742807	H85	11.566077	2.393722	6.994675
H3	14.539943	4.667587	7.757770	H86	14.449157	3.035554	6.105602
C4	12.649446	4.290158	8.828742	73			
H5	12.430170	5.364618	8.912047	3a - TS dis			
H6	11.699029	3.780339	8.649271	N1	11.878812	8.574359	5.699170
H7	13.048979	3.971207	9.802946	N2	11.486850	7.633706	3.651022
Ru9	12.754688	5.399523	5.646041	B3	12.097813	7.329934	4.958338
C110	10.419860	4.851792	6.278427	C4	12.377763	9.010412	6.957747
C111	15.088116	6.142967	5.557521	C5	11.597706	8.868973	8.112402
O12	11.189203	2.651435	2.561863	C6	12.111291	9.330808	9.325256
N13	11.869290	8.399621	5.675232	H7	11.507796	9.219827	10.228879
N14	11.576556	7.574144	3.567444	C8	13.361813	9.935784	9.409571
B15	12.044960	7.171043	4.894341	C9	14.096056	10.104030	8.237665
C16	12.365763	8.728418	6.966363	H10	15.069551	10.597252	8.282214
C17	11.577458	8.506358	8.105807	C11	13.623672	9.655226	7.007152
C18	12.104378	8.831281	9.356865	C12	10.225404	8.273793	8.038644
H19	11.493608	8.658367	10.245992	H13	9.736400	8.299723	9.019570
C20	13.374269	9.385380	9.498593	H14	10.256262	7.234430	7.685959
C21	14.114292	9.643295	8.347826	H15	9.596130	8.821815	7.324766
H22	15.101945	10.101189	8.437104	C16	13.914309	10.389141	10.729948
C23	13.632036	9.327571	7.078639	H17	14.520772	11.297254	10.622471
C24	10.185458	7.973096	7.975938	H18	14.561309	9.622564	11.177660
H25	9.670988	7.986749	8.944316	H19	13.114832	10.599607	11.450672
H26	10.179707	6.946289	7.583700	C20	14.429279	9.849954	5.760025
H27	9.604419	8.572141	7.263129	H21	15.287674	10.505756	5.947432
C28	13.934072	9.691613	10.858021	H22	13.826312	10.282435	4.950891
H29	14.682501	10.492227	10.813156	H23	14.806405	8.879556	5.409352
H30	14.427389	8.813533	11.296988	C24	11.570471	6.971125	2.400377
H31	13.148143	10.001780	11.557998	C25	10.643817	5.978313	2.054110
C32	14.453670	9.619255	5.861276	C26	10.765228	5.361885	0.809199
H33	15.337444	10.213874	6.121097	H27	10.047549	4.585383	0.534694
H34	13.875886	10.162407	5.102847	C28	11.776622	5.700590	-0.087534
H35	14.791604	8.679763	5.401877	C29	12.681666	6.693506	0.280213
C36	11.734783	6.910158	2.324590	H30	13.486847	6.966948	-0.405302
C37	10.663989	6.203963	1.761119	C31	12.597248	7.334286	1.514743
C38	10.867367	5.536025	0.553382	C32	9.578352	5.564541	3.019667
H39	10.037097	4.983309	0.108522	H33	8.831862	4.926471	2.531579
C40	12.103476	5.538016	-0.088308	H34	9.073937	6.433695	3.458781
C41	13.143353	6.270810	0.479289	H35	10.012969	5.014851	3.867767
H42	14.119619	6.283735	-0.010926	C36	11.907374	4.986331	-1.401735
C43	12.979407	6.965861	1.674675	H37	12.461580	5.587127	-2.132622
C44	9.347218	6.133167	2.472561	H38	10.926169	4.750713	-1.832128
H45	8.628618	5.527353	1.906045	H39	12.444989	4.034978	-1.289257
H46	8.915381	7.130979	2.625509	C40	13.624156	8.342606	1.934499
H47	9.461623	5.694547	3.475515	H41	14.371669	8.498439	1.148257
C48	12.335078	4.725224	-1.328088	H42	14.139651	8.005422	2.845745
H49	12.968784	5.254003	-2.051376	H43	13.171862	9.311112	2.184833
H50	11.392858	4.466061	-1.826792	C44	11.210528	9.492338	4.883132
H51	12.849916	3.785420	-1.077434	C45	10.985179	8.943722	3.673959
C52	14.117122	7.727585	2.281594	H46	10.483759	9.360317	2.807052
H53	14.957336	7.799405	1.580857	H47	10.937295	10.473338	5.257741
H54	14.475727	7.238888	3.200758	Ru48	12.882475	5.632229	5.683096
H55	13.812532	8.742566	2.569683	C149	10.714205	5.034133	6.480915
C56	12.375698	4.582343	4.047068	C150	15.010293	6.435834	6.357407
H57	11.321313	4.603218	3.747923	O51	12.151558	2.481413	4.950747
C58	10.442153	1.619167	1.940723	C52	13.296035	4.870056	4.094397
H59	11.053380	0.700190	1.907305	H53	13.227704	5.378981	3.121574
C60	9.245710	1.400501	2.842187	C54	11.381558	1.301744	5.141562
H61	9.566165	1.107814	3.846828	H55	11.940172	0.598595	5.784630
H62	8.583137	0.627922	2.434440	C56	10.121086	1.724230	5.861401
H63	8.684340	2.338555	2.933566	H57	10.359484	2.242985	6.794022
C64	10.021348	2.022794	0.538686	H58	9.494674	0.847812	6.069616
H65	10.880088	2.286962	-0.089429	H59	9.555670	2.430979	5.242272
H66	9.367940	2.902632	0.599252	C60	11.070149	0.655178	3.802305
H67	9.467489	1.210802	0.051327	H61	11.977979	0.367238	3.261291
C68	12.519442	2.789795	2.340851	H62	10.515907	1.371276	3.182468
C69	13.235228	2.028732	1.417373	H63	10.449808	-0.238918	3.939805
H70	12.732946	1.294213	0.792526	C64	13.441791	2.387095	4.548808
C71	14.611286	2.209307	1.292182	C65	14.189628	1.207633	4.561406
H72	15.159926	1.611702	0.565125	H66	13.745435	0.275794	4.901987
C73	15.276630	3.132180	2.088297	C67	15.516088	1.216361	4.138857
H74	16.351887	3.267981	1.991258	H68	16.086667	0.289034	4.162655
C75	14.562569	3.885941	3.012268	C69	16.104361	2.391427	3.690209
H76	15.061273	4.617551	3.648391	H70	17.141520	2.399984	3.360982
C77	13.176954	3.752985	3.151896	C71	15.353084	3.560733	3.669322
C78	11.349964	9.402763	4.848076	H72	15.797987	4.498963	3.337844
C79	11.176246	8.916604	3.602316	C73	14.024367	3.588743	4.099421
H80	11.130520	10.390637	5.239918	73			
H81	10.779310	9.405518	2.718932	3a - P dis			
C82	12.528964	2.056005	6.598561	Ru9	13.150895	5.593813	5.259339
H83	12.381741	1.846097	5.531401	C110	11.655030	4.753927	6.897902
H84	12.803715	1.108641	7.086607	C111	15.306409	6.490873	4.753003

O12	11.374704	2.615384	2.494522	H11	11.867060	8.288516	10.256797
N13	11.790931	8.339905	5.702648	C12	13.639342	9.203918	9.455656
N14	11.297237	7.587191	3.601609	C13	14.271371	9.624224	8.287526
B15	12.048007	7.205488	4.805349	H14	15.245009	10.115124	8.352814
C16	12.342637	8.657022	6.973915	C15	13.707667	9.411261	7.032577
C17	11.619443	8.375328	8.142926	C16	10.415290	7.769711	8.033671
C18	12.186489	8.700676	9.373670	H17	9.970406	7.684844	9.032453
H19	11.631107	8.473456	10.286248	H18	10.433582	6.771582	7.575434
C20	13.435887	9.308846	9.468431	H19	9.748688	8.376252	7.406724
C21	14.103827	9.634072	8.291147	C20	14.300018	9.385453	10.791734
H22	15.065580	10.148804	8.345527	H21	14.911444	10.296120	10.819157
C23	13.573582	9.328675	7.037557	H22	14.967230	8.544300	11.024813
C24	10.254250	7.765525	8.066117	H23	13.563122	9.447550	11.601846
H25	9.800836	7.700170	9.062143	C24	14.439706	9.818538	5.791145
H26	10.308381	6.756589	7.636959	H25	15.281112	10.479692	6.030112
H27	9.590639	8.355083	7.420211	H26	13.787169	10.323380	5.068143
C28	14.044842	9.601837	10.809210	H27	14.834425	8.919219	5.297850
H29	14.763462	10.428447	10.754061	C28	11.447105	7.189020	2.285908
H30	14.584545	8.729647	11.202726	C29	10.385873	6.353212	1.912872
H31	13.280162	9.866200	11.550376	C30	10.442693	5.718414	0.671771
C32	14.282699	9.746522	5.785666	H31	9.623724	5.057743	0.378861
H33	15.122975	10.410824	6.019795	C32	11.520059	5.892120	-0.195230
H34	13.602379	10.272420	5.102653	C33	12.556108	6.739183	0.194915
H35	14.673729	8.875770	5.241914	H34	13.410547	6.883672	-0.470144
C36	11.266946	7.048746	2.291046	C35	12.539126	7.389060	1.427796
C37	10.181755	6.264754	1.883557	C36	9.245695	6.119151	2.854407
C38	10.156339	5.786586	0.571624	H37	8.456451	5.526727	2.376888
H39	9.302852	5.189903	0.239510	H38	8.811774	7.064471	3.204600
C40	11.186302	6.058083	-0.325494	H39	9.587477	5.589371	3.756047
C41	12.258508	6.836210	0.110776	C40	11.583252	5.152587	-1.501066
H42	13.074355	7.058116	-0.580958	H41	12.167055	5.703187	-2.248646
C43	12.316936	7.343590	1.405907	H42	10.582618	4.977051	-1.914298
C44	9.109858	5.904533	2.866345	H43	12.058296	4.168740	-1.382214
H45	8.276898	5.387715	2.374759	C44	13.700525	8.219477	1.884933
H46	8.718694	6.787427	3.385366	H45	14.434721	8.352131	1.081862
H47	9.516646	5.242640	3.645678	H46	14.201438	7.735879	2.736837
C48	11.159450	5.523925	-1.728446	H47	13.386026	9.209062	2.241986
H49	11.341834	6.316199	-2.466091	C48	13.081583	4.806036	3.745101
H50	10.194432	5.059786	-1.964495	H49	12.889578	5.322574	2.795660
H51	11.937243	4.763376	-1.881503	C50	13.766908	2.509793	7.122211
C52	13.476870	8.171919	1.866222	H51	14.682390	1.892255	7.130666
H53	14.128177	8.438279	1.025740	C52	13.855719	3.548067	8.218221
H54	14.078034	7.630206	2.611930	H53	14.705310	4.217787	8.048581
H55	13.137783	9.094895	2.355247	H54	13.960801	3.056843	9.193379
C56	12.742040	4.602926	3.787046	H55	12.942627	4.157866	8.224714
H57	11.979187	4.891475	3.055478	C56	12.526035	1.646378	7.246658
C58	10.662657	1.800748	1.576830	H57	12.466212	0.894511	6.451921
H59	10.734878	0.743669	1.886530	H58	11.641570	2.292400	7.174685
C60	9.219468	2.242290	1.676354	H59	12.519601	1.129563	8.214341
H61	8.853195	2.141950	2.703093	C60	13.906552	2.643163	4.701805
H62	8.584668	1.647406	1.009348	C61	14.380890	1.346012	4.529027
H63	9.143588	3.298017	1.389055	H62	14.618563	0.725897	5.389746
C64	11.216864	1.984803	0.175352	C63	14.556805	0.840038	3.242108
H65	12.270958	1.692231	0.116763	H64	14.930008	-0.175596	3.118768
H66	11.141428	3.046689	-0.095467	C65	14.258958	1.615922	2.128203
H67	10.649331	1.391866	-0.552516	H66	14.395325	1.214424	1.125867
C68	12.636813	2.282410	2.875694	C67	13.780724	2.908371	2.307867
C69	13.214630	1.035063	2.649446	H68	13.533466	3.535539	1.449808
H70	12.677696	0.264220	2.102247	C69	13.591762	3.452871	3.583635
C71	14.490190	0.760595	3.138442	C70	11.276034	9.570210	4.956706
H72	14.928347	-0.219774	2.957070	C71	11.016589	9.150716	3.693987
C73	15.195159	1.725919	3.844145	C72	10.950073	10.868675	5.603680
H74	16.195045	1.515662	4.217872	H73	10.425118	11.530075	4.905354
C75	14.624186	2.975224	4.053847	H74	10.306517	10.733371	6.485789
H76	15.182087	3.760580	4.564382	H75	11.846969	11.399255	5.955839
C77	13.343611	3.288679	3.578132	C76	10.344828	9.866773	2.577708
C78	10.980303	9.274385	5.052374	H77	10.053776	10.877143	2.885648
C79	10.687005	8.833699	3.813723	H78	10.992317	9.962647	1.693149
H80	10.673562	10.188210	5.550523	H79	9.436751	9.345547	2.238361
H81	10.082065	9.293101	3.039551	79			
3b - s				3b - s - cis			
Ru1	12.818463	5.565111	5.382254	Ru1	12.979466	5.541920	5.476794
C12	10.665002	4.734739	6.071424	C12	10.763530	4.697325	5.704846
C13	14.989973	6.388648	5.933195	C13	13.577856	4.671461	7.723879
O4	13.732169	3.245371	5.896643	O4	15.218819	6.055778	4.899682
N5	11.891308	8.524409	5.672288	N5	11.773310	8.402378	5.660867
N6	11.449657	7.814585	3.555491	N6	11.476454	7.676569	3.516233
B7	12.050919	7.346871	4.808188	B7	12.070383	7.262650	4.786091
C8	12.463819	8.763617	6.950040	C8	12.346165	8.758605	6.911316
C9	11.783545	8.375498	8.112249	C9	11.827501	8.251707	8.111329
C10	12.392543	8.594626	9.349287	C10	12.418928	8.653991	9.309254
				H11	12.021379	8.257750	10.245751

C12	13.489733	9.542024	9.346588	N13	11.150512	8.348311	5.448072
C13	13.974466	10.044675	8.140882	N14	10.649627	6.971465	3.703982
H14	14.817274	10.740136	8.147738	B15	11.520849	7.044473	4.883763
C15	13.423460	9.661043	6.920394	C16	11.784562	9.103417	6.470572
C16	10.669284	7.306469	8.117874	C17	11.413311	8.932350	7.809766
H17	10.196819	7.279864	9.106588	C18	12.051912	9.702787	8.783985
H18	10.989802	6.286307	7.863273	H19	11.766105	9.571028	9.830101
H19	9.920754	7.582289	7.366711	C20	13.026047	10.640170	8.456210
C20	14.123404	9.923966	10.652778	C21	13.353756	10.812435	7.112457
H21	14.614187	10.902964	10.592925	H22	14.113190	11.547651	6.836776
H22	14.887075	9.194390	10.953757	C23	12.754124	10.054869	6.111136
H23	13.383757	9.964330	11.461712	C24	10.337778	7.961999	8.192876
C24	13.995707	10.170786	5.630385	H25	10.032295	8.111586	9.235504
H25	14.930667	10.717200	5.804976	H26	10.662167	6.919061	8.072674
H26	13.301680	10.834650	5.098410	H27	9.455191	8.068973	7.549328
H27	14.200077	9.336874	4.942333	C28	13.722175	11.437764	9.520496
C28	11.571236	7.117639	2.215780	H29	13.939606	12.458785	9.182177
C29	10.546016	6.300488	1.721675	H30	14.681617	10.981382	9.798262
C30	10.667709	5.786896	0.428878	H31	13.118335	11.505271	10.433408
H31	9.877475	5.138946	0.043801	C32	13.169241	10.211077	4.680244
C32	11.767084	6.073841	-0.375769	H33	13.825070	11.080625	4.553853
C33	12.759088	6.910517	0.130780	H34	12.311307	10.315306	4.003003
H34	13.635056	7.136842	-0.481812	H35	13.720359	9.312577	4.368202
C35	12.680600	7.436926	1.416563	C36	10.614974	6.024817	2.650795
C36	9.357432	5.983112	2.573504	C37	9.743592	4.929941	2.713590
H37	8.644018	5.351386	2.031706	C38	9.765531	3.999637	1.673344
H38	8.840423	6.898521	2.889840	H39	9.091174	3.140097	1.718755
H39	9.662764	5.469419	3.497738	C40	10.618851	4.138374	0.580302
C40	11.916649	5.465594	-1.739929	C41	11.450007	5.256035	0.525240
H41	12.246052	6.205977	-2.480112	H42	12.120543	5.383899	-0.327530
H42	10.975924	5.028698	-2.093946	C43	11.463585	6.203501	1.546841
H43	12.670531	4.665230	-1.735330	C44	8.824525	4.769273	3.883315
C44	13.778416	8.302721	1.954835	H45	8.131107	3.933047	3.728666
H45	14.581425	8.422959	1.218018	H46	8.236342	5.679072	4.060459
H46	14.212184	7.860140	2.861947	H47	9.397342	4.594311	4.806091
H47	13.408212	9.297107	2.240312	C48	10.665400	3.096127	-0.499357
C48	13.081186	4.913599	3.760029	H49	10.894497	3.537094	-1.477382
H49	12.270452	4.350823	3.268345	H50	9.713032	2.558955	-0.583980
C50	16.346050	6.292317	5.783181	H51	11.442236	2.346688	-0.295411
H51	17.108167	6.824950	5.193176	C52	12.418186	7.359395	-1.522200
C52	15.880726	7.204701	6.889908	H53	12.948703	7.416032	0.564683
H53	15.496717	8.146213	6.485682	H54	13.162978	7.258903	2.325859
H54	16.730618	7.432874	7.546093	H55	11.910520	8.316458	1.701381
H55	15.093943	6.723816	7.484923	C56	10.163468	8.958750	4.649103
C56	16.875087	4.965192	6.283022	C57	9.868416	8.143617	3.608236
H57	17.180384	4.316225	5.453684	Ru58	12.806324	5.722243	5.720111
H58	16.086582	4.465892	6.861062	C159	10.960738	4.658304	6.842426
H59	17.744864	5.129150	6.931161	C160	14.683765	7.220117	5.756542
C60	15.456122	5.566755	3.642505	O61	12.172571	2.398479	4.564068
C61	16.674390	5.649216	2.975741	C62	13.142707	4.797178	4.212738
H62	17.551827	6.073731	3.454510	H63	12.656286	4.940682	3.239165
C63	16.771141	5.181693	1.165542	C64	11.455933	1.171007	4.575675
H64	17.726341	5.256513	1.148428	H65	11.922786	0.487452	5.308270
C65	15.669527	4.624937	1.025405	C66	10.059216	1.517123	5.037774
H66	15.751447	4.267146	0.000386	H67	10.093756	2.063581	5.986955
C67	14.465263	4.521288	1.709281	H68	9.453484	0.609786	5.149505
H68	13.584917	4.091455	1.230049	H69	9.583155	2.173083	4.297657
C69	14.330736	4.985553	3.021935	C70	11.456578	0.549661	3.189148
C70	11.063493	9.366129	4.934580	H71	12.469110	0.314673	2.842586
C71	10.886910	8.938483	3.669431	H72	11.011936	1.264774	2.483567
C72	10.511490	10.579727	5.597090	H73	10.862186	-0.372299	3.175385
H73	9.913910	11.170953	4.894564	C74	13.524370	2.386822	4.480245
H74	9.861427	10.308743	6.442776	C75	14.344767	1.265966	4.590957
H75	11.290278	11.238691	6.008751	H76	13.923732	0.271946	4.722330
C76	10.169910	9.605932	2.549075	C77	15.730255	1.430206	4.549606
H77	9.779512	10.579851	2.863657	H78	16.369626	0.552878	4.638081
H78	10.825268	9.775752	1.681791	C79	16.293593	2.691979	4.408736
H79	9.321534	9.010459	2.179313	H80	17.375275	2.810913	4.390104
91				C81	15.465167	3.808696	4.303353
3b - TS inter				H82	15.876534	4.814998	4.229967
C1	14.319613	3.435733	7.716317	C83	14.080903	3.668440	4.320766
C2	14.427686	4.696415	8.155857	C84	9.558120	10.265294	5.021164
H3	15.229097	5.305308	7.732723	H85	8.765633	10.540241	4.316214
C4	13.572572	5.382194	9.173879	H86	9.115866	10.234481	6.027971
H5	14.108775	5.507966	10.126626	H87	10.293467	11.083149	5.033417
H6	13.309828	6.393624	8.830762	C88	8.873993	8.327660	2.517967
H7	12.636441	4.847824	9.366677	H89	8.352396	9.284556	2.629741
C8	13.294210	2.420268	8.098956	H90	9.340088	8.318353	1.521242
H9	12.580248	2.279814	7.272779	H91	8.113709	7.531906	2.508199
H10	13.761843	1.447040	8.305217	91			
H11	12.710348	2.716727	8.976785	3b - P inter			
H12	15.036892	3.111592	6.958735	C1	13.824534	3.125066	6.042180

C2	13.867389	3.949959	7.111328	C86	10.918659	10.773787	5.797527
H3	14.688333	4.670675	7.138194	H87	10.412840	11.496625	5.147519
C4	12.966949	3.931951	8.304442	H88	10.279228	10.611520	6.678367
H5	12.643818	4.950303	8.562400	H89	11.840128	11.246799	6.168175
H6	12.064375	3.337046	8.138802	C89	10.212788	9.966620	2.732474
H7	13.498770	3.533286	9.181196	H90	9.981715	10.974712	3.094551
Ru9	12.719556	5.459138	5.235467	H91	10.845494	10.070666	1.838226
C110	10.500047	4.700108	6.042446	H92	9.271096	9.509390	2.392218
C111	15.015019	6.286891	4.960478	79			
O12	11.021152	2.832162	2.130937	3b	- TS dis		
N13	11.783970	8.400485	5.709640	N1	11.873786	8.606097	5.723564
N14	11.259421	7.824647	3.569186	N2	11.474196	7.653916	3.687305
B15	11.877584	7.278755	4.774215	B3	12.095571	7.360413	4.983222
C16	12.425518	8.537457	6.970805	C4	12.459738	9.040191	6.944887
C17	11.776359	8.119434	8.143269	C5	11.788728	8.852607	8.159878
C18	12.449831	8.235010	9.360569	C6	12.401371	9.289312	9.335719
H19	11.947572	7.905160	10.272967	H7	11.884561	9.137479	10.285943
C20	13.731655	8.772512	9.443077	C8	13.643918	9.915246	9.327859
C21	14.330810	9.232225	8.273159	C9	14.268524	10.129823	8.101208
H22	15.325228	9.681602	8.321590	H10	15.237836	10.632604	8.074611
C23	13.701028	9.126037	7.034133	C11	13.698268	9.701195	6.906087
C24	10.377154	7.589988	8.095435	C12	10.430713	8.221855	8.198297
H25	9.970148	7.474624	9.107313	H13	10.028348	8.227094	9.218249
H26	10.329855	6.619203	7.581563	H14	10.457983	7.185429	7.837119
H27	9.720583	8.262867	7.529205	H15	9.724507	8.753181	7.546140
C28	14.453489	8.847674	10.757737	C16	14.307978	10.333445	10.607700
H29	15.165097	9.682218	10.778941	H17	14.889311	11.255036	10.478268
H30	15.026913	7.931197	10.953723	H18	15.004183	9.562888	10.965798
H31	13.755869	8.975550	11.594709	H19	13.575293	10.504299	11.405704
C32	14.382031	9.619607	5.795117	C20	14.408506	9.908221	5.604086
H33	15.252825	10.236186	6.047878	H21	15.264369	10.582250	5.727112
H34	13.707137	10.206369	5.159651	H22	13.746104	10.315520	4.828795
H35	14.724781	8.765021	5.194804	H23	14.783479	8.941337	5.240595
C36	11.280107	7.271670	2.264012	C24	11.527299	6.933123	2.467991
C37	10.186381	6.534044	1.790884	C25	10.575895	5.945518	2.180284
C38	10.267635	5.962105	0.520724	C26	10.671073	5.261391	0.968280
H39	9.420274	5.383329	0.146814	H27	9.933046	4.488784	0.740589
C40	11.404662	6.090178	-0.273046	C28	11.678295	5.532299	0.045121
C41	12.468898	6.847844	0.211481	C29	12.610614	6.521183	0.353694
H42	13.372487	6.951819	-0.393811	H30	13.414646	6.739695	-0.352667
C43	12.426002	7.444504	1.468938	C31	12.554971	7.223590	1.555834
C44	8.983598	6.315713	2.658249	C32	9.506443	5.613393	3.172546
H45	8.238345	5.696875	2.142417	H33	8.785828	4.901575	2.751018
H46	8.507466	7.263282	2.944314	H34	8.965659	6.510550	3.500022
H47	9.258360	5.817268	3.600512	H35	9.942801	5.180020	4.084389
C48	11.514103	5.380293	-1.590597	C36	11.781782	4.752469	-1.233724
H49	12.014569	5.997705	-2.347405	H37	12.219781	5.354793	-2.038971
H50	10.529167	5.095577	-1.981313	H38	10.799845	4.399288	-1.570928
H51	12.108840	4.460228	-1.481734	H39	12.418580	3.866088	-1.111298
C52	13.599555	8.210383	1.998548	C40	13.616692	8.217020	1.921768
H53	14.349573	8.370737	1.215049	H41	14.346323	8.333962	1.112275
H54	14.078076	7.666976	2.828711	H42	14.150729	7.885958	2.824955
H55	13.300830	9.186745	2.403723	H43	13.199410	9.203546	2.163988
C56	12.213320	4.768499	3.610767	C44	11.198076	9.532384	4.904820
H57	11.131345	4.718111	3.439156	C45	10.960060	8.970622	3.695035
C58	10.269185	1.829006	1.468530	Ru46	12.928113	5.671972	5.702292
H59	10.927848	0.973339	1.237759	C147	10.804084	5.020089	6.575540
C60	9.215900	1.398377	2.466829	C148	15.040960	6.541075	6.347627
H61	9.681623	1.005867	3.376124	O49	11.994596	2.623963	4.787738
H62	8.560837	0.631183	2.037236	C50	13.344229	4.897502	4.125440
H63	8.608720	2.265994	2.752301	H51	13.255066	5.362478	3.133676
C64	9.647285	2.373467	0.194897	C52	11.112180	1.508049	4.785728
H65	10.401599	2.772108	-0.493413	H53	11.523392	0.712422	5.431699
H66	8.962266	3.191594	0.452453	C54	9.805666	1.982772	5.379441
H67	9.078147	1.592354	-0.324404	H55	9.963132	2.410599	6.373203
C68	12.285621	3.134552	1.745153	H56	9.095695	1.148262	5.437568
C69	12.930607	2.530580	0.665925	H57	9.374287	2.774106	4.754090
H70	12.416287	1.798886	0.047712	C58	10.930247	0.993787	3.367971
C71	14.252255	2.863129	0.375872	H59	11.876219	0.660700	2.926958
H72	14.745160	2.386839	-0.470943	H60	10.531001	1.806521	2.746852
C73	14.935227	3.781802	1.161450	H61	10.222198	0.156261	3.345239
H74	15.969365	4.036080	0.937673	C62	13.311439	2.429175	4.537921
C75	14.292189	4.379091	2.239262	C63	13.965057	1.197339	4.606957
H76	14.809373	5.100494	2.871438	H64	13.417218	0.291126	4.852818
C77	12.957752	4.094695	2.548392	C65	15.333951	1.123792	4.363835
C78	11.185986	9.505586	5.068786	H66	15.832892	0.157882	4.429288
C79	10.876060	9.163787	3.793086	C67	16.057531	2.265853	4.045977
C82	12.847234	2.017138	5.807149	H68	17.128951	2.207243	3.864569
H83	12.650783	1.900054	4.734075	C69	15.399035	3.487955	3.962515
H84	13.237140	1.057265	6.178360	H70	15.947503	4.400377	3.730619
H85	11.885895	2.219381	6.290867	C71	14.027550	3.592761	4.200530
H86	14.607587	3.257104	5.292084	C72	10.811150	10.875820	5.411218

H73	10.278683	11.443781	4.640324
H74	10.157164	10.809484	6.293453
H75	11.684361	11.468934	5.719673
C76	10.216261	9.518190	2.529853
H77	9.872789	10.537789	2.736340
H78	10.829131	9.553281	1.616810
H79	9.332828	8.909778	2.283455
79			
3b - P dis			
Ru9	13.051656	5.685282	4.823172
Cl10	11.732292	4.547304	6.437390
Cl11	15.131241	6.717111	4.255023
O12	11.124606	2.966380	1.927411
N13	11.724982	8.337270	5.733603
N14	11.042983	7.846007	3.612869
B15	11.888874	7.321885	4.688003
C16	12.433482	8.482336	6.957939
C17	11.886878	7.993361	8.154191
C18	12.615122	8.146931	9.333924
H19	12.196595	7.758798	10.265048
C20	13.852492	8.784740	9.355858
C21	14.343875	9.315325	8.165698
H22	15.294939	9.852364	8.170967
C23	13.651921	9.182860	6.962807
C24	10.537041	7.345333	8.171759
H25	10.208147	7.160913	9.201354
H26	10.562435	6.388073	7.634717
H27	9.784539	7.970128	7.673062
C28	14.641420	8.893791	10.628684
H29	15.251332	9.805484	10.648109
H30	15.328492	8.044761	10.747172
H31	13.987417	8.904126	11.509260
C32	14.184623	9.799425	5.705192
H33	15.024572	10.468556	5.926565
H34	13.411413	10.373139	5.176818
H35	14.536132	9.024376	5.010198
C36	10.909099	7.418474	2.268589
C37	9.840689	6.593398	1.897126
C38	9.730190	6.198097	0.562273
H39	8.889068	5.567120	0.263098
C40	10.664633	6.584030	-0.394891
C41	11.721951	7.401791	0.003241
H42	12.465816	7.710902	-0.734648
C43	11.861293	7.829669	1.320977
C44	8.892500	6.079946	2.937111
H45	8.028227	5.585132	2.477645
H46	8.533121	6.876726	3.598623
H47	9.403203	5.350350	3.583918
C48	10.558450	6.118862	-1.818665
H49	10.715913	6.942330	-2.526987
H50	9.575582	5.678980	-2.026655
H51	11.315073	5.355229	-2.047318
C52	13.021767	8.677346	1.744021
H53	13.584601	9.036993	0.874788
H54	13.707187	8.104444	2.387422
H55	12.696846	9.543430	2.336162
C56	12.558973	4.860772	3.276145
H57	11.736897	5.202422	2.639328
C58	10.308680	2.137360	1.115699
H59	10.466357	1.080901	1.393758
C60	8.881844	2.519849	1.440412
H61	8.678952	2.387335	2.507994
H62	8.176419	1.911108	0.862757
H63	8.722249	3.576545	1.192828
C64	10.635851	2.355771	-0.350993
H65	11.681816	2.116168	-0.571194
H66	10.469945	3.413298	-0.597000
H67	9.994631	1.739157	-0.992963
C68	12.423151	2.635018	2.159070
C69	13.004909	1.431444	1.765866
H70	12.437541	0.694458	1.203392
C71	14.328943	1.156031	2.103081
H72	14.769340	0.209882	1.791767
C73	15.077832	2.076975	2.821572
H74	16.114239	1.866176	3.076759
C75	14.500712	3.283426	3.200152
H76	15.085689	4.037072	3.728064
C77	13.172783	3.595605	2.881348
C78	10.885896	9.369769	5.269590
C79	10.479263	9.080565	4.009760
C86	10.544863	10.537892	6.124036
H87	9.873567	11.223129	5.594757

H88	10.047004	10.235839	7.057535
H89	11.437173	11.107709	6.422190
C89	9.582140	9.848602	3.106703
H90	9.240034	10.768050	3.594333
H91	10.082966	10.134995	2.169723
H92	8.690137	9.274051	2.814677
79			
3c - S			
Ru1	12.873457	5.591725	5.376849
Cl2	10.718947	4.790103	6.088282
Cl3	15.060436	6.392061	5.891507
O	13.761413	3.288519	5.912473
N5	11.971456	8.534078	5.685236
N6	11.520676	7.829106	3.541093
B7	12.127091	7.358260	4.801516
C10	12.516963	8.760945	6.979077
C11	11.793785	8.396350	8.120757
C12	12.377598	8.603477	9.372106
H13	11.821161	8.315597	10.266739
C14	13.636757	9.180033	9.506181
C15	14.306294	9.587703	8.354040
H16	15.285359	10.063179	8.443491
C17	13.766879	9.391775	7.086589
C18	10.406587	7.843719	8.002812
H19	9.938750	7.755300	8.990429
H20	10.396776	6.855722	7.523650
H21	9.780839	8.496762	7.380794
C22	14.269858	9.352167	10.856207
H23	14.840117	10.287567	10.918141
H24	14.970458	8.535026	11.075496
H25	13.518727	9.359266	11.654618
C26	14.508284	9.826518	5.860911
H27	15.419346	10.373322	6.129923
H28	13.891849	10.471545	5.221880
H29	14.797870	8.946671	5.271373
C30	11.479864	7.207533	2.267993
C31	10.385060	6.411395	1.910686
C32	10.403524	5.779574	0.666797
H33	9.559516	5.147086	0.383742
C34	11.472527	5.924422	-0.215210
C35	12.538189	6.742049	0.158853
H36	13.382267	6.869172	-0.522606
C37	12.559869	7.390127	1.392039
C38	9.247063	6.226517	2.865433
H39	8.442991	5.638214	2.408608
H40	8.835503	7.193768	3.181469
H41	9.581165	5.714442	3.779777
C42	11.496574	5.190285	-1.525002
H43	12.038566	5.754579	-2.293683
H44	10.484023	4.995241	-1.897613
H45	11.997173	4.217183	-1.427529
C46	13.737260	8.213122	1.819345
H47	14.468456	8.307539	1.008420
H48	14.237729	7.752662	2.683849
H49	13.433576	9.220046	2.133947
C50	13.108689	4.818090	3.741649
H51	12.898888	5.320015	2.787963
C52	13.793890	2.569395	7.149374
H53	14.711776	1.956287	7.168674
C54	13.874976	3.622935	8.231457
H55	14.724725	4.291348	8.057618
H56	13.976263	3.145070	9.213433
H57	12.960225	4.230277	8.226831
C58	12.555605	1.703619	7.279157
H59	12.501185	0.942010	6.493351
H60	11.669263	2.345656	7.197251
H61	12.547323	1.198427	8.252806
C62	13.942551	2.672816	4.725747
C63	14.426395	1.377157	4.570531
H64	14.666894	0.769763	5.439323
C65	14.609319	0.857440	3.290423
H66	14.991133	-0.156376	3.180462
C67	14.308538	1.616775	2.165632
H68	14.451282	1.203639	1.169117
C69	13.820031	2.907482	2.327522
H70	13.570496	3.522001	1.461116
C71	13.624763	3.465828	3.596449
C72	11.338155	9.563439	5.003086
C73	11.066372	9.135275	3.688688
C74	10.449648	9.982214	2.779844
C75	10.097916	11.269244	3.202958
C76	10.362120	11.691920	4.502415

C77	10.988252	10.840163	5.419187	H80	10.126797	9.427627	1.697092
H80	10.252117	9.643109	1.763315	H81	9.275828	11.660627	2.438710
H81	9.613222	11.946951	2.501716	H82	9.649809	12.434770	4.759815
H82	10.082858	12.697895	4.811490	H83	10.892073	10.994681	6.388990
H83	11.210153	11.160496	6.436622	91			
79				3c - TS inter			
3c - S - cis				C1	14.268146	3.574320	7.703712
Ru1	13.020608	5.583535	5.451067	C2	14.345096	4.889800	7.959533
C12	10.776337	4.833428	5.712841	H3	15.152114	5.444371	7.479986
C13	13.586128	4.670956	7.683744	C4	13.498064	5.683829	8.904895
O	15.292976	5.949500	4.863200	H5	14.045378	5.887364	9.837023
N5	11.896707	8.451603	5.633744	H6	13.248892	6.668041	8.478717
N6	11.529380	7.719135	3.480812	H7	12.558392	5.180800	9.156517
B7	12.147293	7.304601	4.747359	C8	13.286049	2.599768	8.266185
C10	12.508741	8.749452	6.883699	H9	12.385550	3.097722	8.641843
C11	11.951456	8.288341	8.082540	H10	12.963581	1.892367	7.490313
C12	12.609410	8.590625	9.275920	H11	13.728288	2.010380	9.083687
H13	12.189202	8.219183	10.212350	H12	15.006164	3.161905	7.010909
C14	13.779876	9.341286	9.305050	N13	11.142233	8.200762	5.423851
C15	14.290473	9.821380	8.099380	N14	10.706283	6.839438	3.612095
H16	15.206039	10.417952	8.102735	B15	11.554460	6.913742	4.820881
C17	13.675796	9.532238	6.884282	C16	11.728609	8.957040	6.479513
C18	10.686813	7.490895	8.089806	C17	11.266435	8.818030	7.794390
H19	10.244601	7.475009	9.092426	C18	11.869133	9.581581	8.796621
H20	10.869689	6.453362	7.775784	H19	11.516739	9.471560	9.824558
H21	9.954977	7.900237	7.383477	C20	12.887903	10.486878	8.516906
C22	14.497069	9.602597	10.597721	C21	13.284798	10.647663	7.190927
H23	14.989918	10.582841	10.596383	H22	14.062340	11.375429	6.949377
H24	15.275903	8.848994	10.777679	C23	12.717661	9.902806	6.160925
H25	13.811539	9.567532	11.452594	C24	10.119268	7.910774	8.115856
C26	14.257652	10.022330	5.591521	H25	9.837745	8.001436	9.171605
H27	15.220351	10.520976	5.757820	H26	10.354457	6.859862	7.903023
H28	13.586752	10.728778	5.084107	H27	9.242647	8.158178	7.502332
H29	14.415775	9.187883	4.892192	C28	13.547557	11.272511	9.612778
C30	11.556158	7.114759	2.195922	H29	13.839776	12.273221	9.270833
C31	10.476723	6.336361	1.757121	H30	14.460641	10.775450	9.966532
C32	10.540364	5.771132	0.482058	H31	12.885788	11.390324	10.479226
H33	9.709048	5.151052	0.140467	C32	13.146663	10.110829	4.741143
C34	11.631156	5.973815	-0.359025	H33	13.858248	10.941505	4.667906
C35	12.675344	6.779224	0.091084	H34	12.290293	10.329945	4.089497
H36	13.543485	6.943110	-0.551863	H35	13.636452	9.204354	4.362111
C37	12.656261	7.355093	1.358059	C36	10.756140	5.973004	2.488638
C38	9.292918	6.113595	2.644362	C37	9.981054	4.807135	2.453966
H39	8.535624	5.502382	2.140209	C38	10.067063	3.985174	1.330464
H40	8.832264	7.067081	2.934380	H39	9.464678	3.073906	1.296159
H41	9.591911	5.614192	3.577791	C40	10.891963	4.297295	0.251032
C42	11.714647	5.310991	-1.702930	C41	11.632197	5.476144	0.302205
H43	12.056896	6.008251	-2.478172	H42	12.280131	5.739927	-0.536360
H44	10.745833	4.905448	-2.015753	C43	11.577586	6.324280	1.407111
H45	12.430986	4.477252	-1.687373	C44	9.091035	4.464545	3.605912
C46	13.802660	8.193483	1.833927	H45	8.529396	3.542595	3.408743
H47	14.575215	8.276972	1.060536	H46	8.374148	5.272126	3.805500
H48	14.264637	7.751278	2.727326	H47	9.675768	4.341603	4.529443
H49	13.474382	9.204007	2.113894	C48	10.995640	3.371341	-0.926149
C50	13.077913	4.935026	3.739369	H49	11.353448	3.895957	-1.819845
H51	12.232562	4.419877	3.254445	H50	10.027412	2.915054	-1.166594
C52	16.442116	6.088276	5.742459	H51	11.697296	2.549649	-0.728388
H53	17.239051	6.565676	5.151653	C52	12.421003	7.561959	1.476572
C54	16.057517	7.024173	6.859757	H53	12.992644	7.701765	0.552049
H55	15.758682	8.000685	6.466668	H54	13.130570	7.505384	2.315431
H56	16.923381	7.168597	7.518905	H55	11.810088	8.458540	1.645899
H57	15.231532	6.606899	7.449559	Ru56	12.816882	5.597449	5.661438
C58	16.870301	4.719149	6.224783	C157	10.889909	4.679271	6.785525
H59	17.116720	4.056631	5.386660	C158	14.704661	7.106913	5.517364
H60	16.051569	4.276394	6.806488	O59	12.284732	2.372412	5.100933
H61	17.756552	4.808923	6.865021	C60	13.173406	4.730034	4.117680
C62	15.488446	5.441322	3.606523	H61	12.910378	5.077312	3.108742
C63	16.704442	5.447765	2.929904	C62	11.510612	1.176507	5.041742
H64	17.609027	5.821858	3.399795	H63	12.056473	0.356466	5.542898
C65	16.763396	4.969455	1.621833	C64	10.236948	1.439795	5.811383
H66	17.717222	4.985225	1.097165	H65	10.458297	1.757615	6.835078
C67	15.626038	4.475789	0.992135	H66	9.620303	0.532411	5.832975
H68	15.678820	4.107862	-0.031075	H67	9.668092	2.248236	5.338305
C69	14.423471	4.446983	1.685431	C68	11.242455	0.817254	3.591015
H70	13.516167	4.067265	1.215298	H69	12.171631	0.607051	3.048635
C71	14.326726	4.925768	2.996452	H70	10.747608	1.667308	3.100246
C72	11.180140	9.425606	4.947740	H71	10.590686	-0.062206	3.517589
C73	10.960033	8.981309	3.630022	C72	13.570651	2.337978	4.672611
C74	10.282157	9.777178	2.717282	C73	14.400144	1.217769	4.726890
C75	9.812526	11.025285	3.141360	H74	14.022967	0.266322	5.095099
C76	10.023925	11.461253	4.447173	C75	15.727976	1.322880	4.319966
C77	10.713931	10.663396	5.366465	H76	16.371268	0.445707	4.374145

C77 16.232093 2.531441 3.853407  
H78 17.272342 2.610419 3.543489  
C79 15.394941 3.640396 3.782505  
H80 15.768284 4.601375 3.429696  
C81 14.061148 3.559945 4.184351  
C82 10.146410 8.785771 4.652489  
C83 9.882084 7.959350 3.545327  
C84 8.937908 8.321991 2.596112  
C85 8.249418 9.527012 2.770274  
C86 8.509054 10.343969 3.866191  
C87 9.464415 9.982450 4.821070  
H88 8.750407 7.678921 1.736877  
H89 7.504669 9.828126 2.035098  
H90 7.966038 11.280713 3.982907  
H91 9.685646 10.620238 5.676214  
91  
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C1 13.638531 3.146773 6.783309  
C2 13.679940 4.116803 7.723023  
H3 14.566103 4.755432 7.723857  
C4 12.686640 4.371553 8.811187  
H5 12.448567 5.443511 8.875740  
H6 11.744576 3.840440 8.651014  
H7 13.100711 4.078760 9.787443  
Ru9 12.781943 5.435888 5.604150  
C110 10.457541 4.882056 6.255478  
C111 15.123508 6.138993 5.471141  
O12 11.207953 2.577984 2.657854  
N13 11.908120 8.421664 5.650131  
N14 11.623564 7.603173 3.515757  
B15 12.078477 7.194284 4.852990  
C16 12.364798 8.698353 6.969750  
C17 11.521457 8.480761 8.069409  
C18 12.016607 8.739815 9.348660  
H19 11.365709 8.568342 10.208842  
C20 13.305927 9.224943 9.553575  
C21 14.097967 9.490434 8.439449  
H22 15.098642 9.904656 8.579068  
C23 13.648058 9.244312 7.143523  
C24 10.111529 8.020258 7.871933  
H25 9.554388 8.060914 8.815417  
H26 10.074888 6.992760 7.482723  
H27 9.596277 8.650686 7.136021  
C28 13.830991 9.455791 10.941278  
H29 14.603982 10.233748 10.953729  
H30 14.284000 8.544754 11.355664  
H31 13.032733 9.759784 11.629544  
C32 14.507879 9.573006 5.962559  
H33 15.425187 10.082028 6.280266  
H34 13.979432 10.223232 5.253542  
H35 14.792336 8.657454 5.426658  
C36 11.762512 6.908128 2.285618  
C37 10.684384 6.184457 1.760071  
C38 10.877594 5.471474 0.576818  
H39 10.044691 4.899736 0.162133  
C40 12.107135 5.452673 -0.076839  
C41 13.151647 6.209118 0.450671  
H42 14.122103 6.205874 -0.050717  
C43 13.000420 6.945966 1.622686  
C44 9.374662 6.140216 2.486343  
H45 8.646910 5.525411 1.942014  
H46 8.952397 7.145605 2.615177  
H47 9.493920 5.723347 3.498011  
C48 12.326671 4.593497 -1.287181  
H49 12.952101 5.094560 -2.036710  
H50 11.379349 4.315369 -1.765317  
H51 12.844332 3.664000 -1.005763  
C52 14.141215 7.731259 2.192239  
H53 14.981565 7.763866 1.489152  
H54 14.498252 7.284793 3.133360  
H55 13.842318 8.762303 2.424259  
C56 12.397133 4.587869 4.021320  
H57 11.339837 4.595635 3.732272  
C58 10.448510 1.537767 2.063135  
H59 11.062387 0.621246 2.017475  
C60 9.280014 1.316653 2.999695  
H61 9.631705 1.032621 3.996516  
H62 8.613475 0.535190 2.616097  
H63 8.712715 2.249727 3.101585  
C64 9.989416 1.934960 0.671647  
H65 10.831949 2.188985 0.017799  
H66 9.343641 2.819470 0.745909

H67 9.416862 1.123776 0.205109  
C68 12.526074 2.733254 2.385256  
C69 13.226974 1.952462 1.466633  
H70 12.720116 1.187133 0.884147  
C71 14.595155 2.151231 1.293780  
H72 15.132089 1.537112 0.571824  
C73 15.268295 3.111827 2.036904  
H74 16.337647 3.261074 1.902409  
C75 14.569417 3.886061 2.955586  
H76 15.074956 4.646176 3.551178  
C77 13.190852 3.736228 3.140561  
C82 12.584400 2.099443 6.617304  
H83 12.426631 1.878040 5.554114  
H84 12.881033 1.160716 7.109039  
H85 11.621810 2.424218 7.024460  
H86 14.489219 3.095607 6.099405  
C87 11.238276 8.939332 3.537638  
C88 11.407376 9.437892 4.845453  
C89 11.102973 10.757809 5.146178  
C90 10.629542 11.583174 4.120266  
C91 10.472075 11.092663 2.827151  
C92 10.778077 9.761926 2.520339  
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H96 10.388728 12.622491 4.337870  
H97 10.110468 11.751839 2.039279  
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79  
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B3 12.150479 7.339092 4.994215  
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C5 11.745813 8.871604 8.158658  
C6 12.325870 9.310921 9.349962  
H7 11.777228 9.173604 10.284271  
C8 13.575599 9.922777 9.375171  
C9 14.237446 10.128420 8.166625  
H10 15.208083 10.628727 8.166146  
C11 13.698761 9.702616 6.956127  
C12 10.374884 8.269100 8.149236  
H13 9.936126 8.286179 9.153712  
H14 10.394632 7.230908 7.792843  
H15 9.708968 8.821361 7.472750  
C16 14.206038 10.341562 10.671762  
H17 14.800529 11.256174 10.554121  
H18 14.883195 9.565723 11.054067  
H19 13.452147 10.524665 11.446853  
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H21 15.303789 10.571302 5.825653  
H22 13.782706 10.404499 4.915920  
H23 14.774064 8.972528 5.261638  
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C25 10.548953 5.872794 2.237283  
C26 10.604072 5.171297 1.032619  
H27 9.855261 4.400078 0.838004  
C28 11.581390 5.428991 10.073937  
C29 12.519866 6.425765 0.334430  
H30 13.293658 6.640980 -0.405498  
C31 12.504009 7.146896 1.526063  
C32 9.499396 5.578178 3.261874  
H33 8.782262 4.837379 2.886705  
H34 8.949071 6.487211 3.538384  
H35 9.950510 5.198795 4.190796  
C36 11.641537 4.634724 -1.198504  
H37 12.050681 5.228990 -2.024497  
H38 10.648996 4.277205 -1.497500  
H39 12.283664 3.750812 -1.087910  
C40 13.552965 8.175353 1.825162  
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H42 14.118478 7.901959 2.728009  
H43 13.109977 9.160556 2.021827  
C44 11.193988 9.478132 4.935558  
C45 10.941194 8.869701 3.691778  
C46 10.243195 9.541328 2.698563  
C47 9.795161 10.840500 2.961943  
C48 10.050136 11.444404 4.189656  
C49 10.755751 10.769607 5.191516  
H50 10.059189 9.059839 1.738763  
H51 9.245560 11.383071 2.194604  
H52 9.699839 12.458520 4.376245  
H53 10.969365 11.236688 6.152291  
Ru54 13.005815 5.690356 5.720872

C155	10.916635	5.017914	6.651217
C156	15.122465	6.566248	6.331981
O57	12.007259	2.681376	4.747658
C58	13.404426	4.921186	4.136930
H59	13.298412	5.387621	3.148109
C60	11.086406	1.598063	4.676028
H61	11.462548	0.753868	5.280118
C62	9.790752	2.084913	5.283397
H63	9.951338	2.449752	6.301572
H64	9.051575	1.274248	5.288585
H65	9.393661	2.923667	4.698504
C66	10.904881	1.173148	3.229306
H67	11.843399	0.825949	2.782970
H68	10.550614	2.037094	2.651093
H69	10.162973	0.369280	3.148327
C70	13.318176	2.454787	4.496941
C71	13.938641	1.204951	4.535667
H72	13.365707	0.307108	4.753801
C73	15.306830	1.104131	4.297787
H74	15.780590	0.124297	4.337548
C75	16.062485	2.235401	4.016556
H76	17.133064	2.153471	3.840026
C77	15.437161	3.476479	3.964408
H78	16.009464	4.380597	3.759824
C79	14.067152	3.606579	4.194460
79			
3c - P dis			
Ru9	13.121531	5.597273	5.246206
C110	11.550462	4.788000	6.826449
C111	15.317868	6.420754	4.810664
O12	11.328944	2.627897	2.524175
N13	11.889335	8.392856	5.619245
N14	11.441474	7.637058	3.484764
B15	12.113606	7.231874	4.735310
C16	12.395271	8.657236	6.923048
C17	11.607068	8.381386	8.050057
C18	12.133800	8.651098	9.311981
H19	11.528733	8.428880	10.193485
C20	13.401985	9.203254	9.475614
C21	14.133738	9.530103	8.336952
H22	15.111202	10.004675	8.445853
C23	13.647136	9.278544	7.054291
C24	10.215238	7.851656	7.896689
H25	9.715688	7.785654	8.870173
H26	10.228632	6.852378	7.443643
H27	9.617202	8.501303	7.244023
C28	13.962580	9.439734	10.848211
H29	14.707433	10.244605	10.846497
H30	14.458532	8.540337	11.237879
H31	13.175509	9.707560	11.564082
C32	14.419193	9.706139	5.843559
H33	15.311913	10.272265	6.133897
H34	13.805352	10.341873	5.191094
H35	14.741166	8.840483	5.249502
C36	11.409420	7.047459	2.194391
C37	10.299625	6.291789	1.801322
C38	10.277358	5.761265	0.509484
H39	9.405399	5.186803	0.186749
C40	11.330550	5.957952	-0.380201
C41	12.425747	6.711305	0.043225
H42	13.259576	6.874874	-0.643034
C43	12.483247	7.269212	1.317413
C44	9.193804	6.024208	2.775618
H45	8.352167	5.515705	2.290577
H46	8.825064	6.950676	3.232171
H47	9.553715	5.388037	3.598121
C48	11.297891	5.384067	-1.767624
H49	11.431710	6.164074	-2.528733
H50	10.346942	4.877640	-1.971536
H51	12.102843	4.651980	-1.918663
C52	13.663320	8.076110	1.765117
H53	14.358447	8.249008	0.935688
H54	14.209085	7.565793	2.572966
H55	13.349991	9.050147	2.164376
C56	12.739450	4.600491	3.770800
H57	12.008308	4.896667	3.011598
C58	10.584131	1.801581	1.642852
H59	10.624610	0.756280	1.994912
C60	9.157281	2.294911	1.733176
H61	8.796238	2.249640	2.765490
H62	8.497918	1.694425	1.096095
H63	9.113071	3.339734	1.402543

C64	11.135402	1.912399	0.232795
H65	12.177412	1.578855	0.178417
H66	11.097921	2.965434	-0.077072
H67	10.541108	1.314883	-0.469201
C68	12.577449	2.265858	2.919161
C69	13.121828	0.998142	2.726252
H70	12.567055	0.228878	2.195145
C71	14.387196	0.702388	3.229269
H72	14.799618	-0.293445	3.074028
C73	15.115415	1.664064	3.915997
H74	16.107158	1.435067	4.299970
C75	14.577766	2.933018	4.093889
H76	15.152774	3.715129	4.590287
C77	13.309511	3.267647	3.601705
C87	10.906824	8.914862	3.637393
C88	11.181754	9.373628	4.939431
C89	10.771154	10.634028	5.348775
C90	10.075527	11.434675	4.437086
C91	9.804872	10.981843	3.149861
C92	10.221253	9.712389	2.733421
H95	10.999216	10.981185	6.356010
H96	9.746771	12.427281	4.741394
H97	9.266245	11.622305	2.453131
H98	10.023460	9.351812	1.724667
74			
3a Na+ - S			
Ru1	13.289562	5.758172	5.177441
C12	11.286578	4.914872	6.114782
C13	15.550796	6.753027	5.263050
O4	14.397101	3.596482	5.681909
N5	12.106595	8.581598	5.558929
N6	12.373138	8.185810	3.321115
B7	12.451394	7.483645	4.620332
C8	11.742691	8.464253	6.939919
C9	10.417775	8.124115	7.258043
C10	10.075667	7.959407	8.596390
H11	9.050639	7.680773	8.845834
C12	11.005297	8.121787	9.621026
C13	12.298574	8.503531	9.279870
H14	13.032258	8.671694	10.069834
C15	12.683797	8.686676	7.951496
C16	9.397713	7.898353	6.185543
H17	8.392626	7.828999	6.613986
H18	9.610700	6.952895	5.667924
H19	9.397127	8.698636	5.434928
C20	10.618142	7.880407	11.049678
H21	11.308813	8.370386	11.744478
H22	10.625014	6.807825	11.282600
H23	9.606695	8.246797	11.260148
C24	14.080453	9.144394	7.646231
H25	14.608594	9.420366	8.564572
H26	14.072493	10.045389	7.010525
H27	14.675648	8.358954	7.157902
C28	12.359322	7.626457	2.007835
C29	11.198555	6.969715	1.570296
C30	11.198731	6.392952	0.302409
H31	10.301769	5.874266	-0.040066
C32	12.313292	6.450388	-0.533725
C33	13.445959	7.120195	-0.076671
H34	14.327147	7.178425	-0.717403
C35	13.488839	7.708031	1.186904
C36	10.011541	6.836056	2.474936
H37	9.157729	6.406260	1.941379
H38	9.704748	7.802945	2.893905
H39	10.243375	6.180609	3.327880
C40	12.294814	5.783950	-1.877337
H41	13.024874	6.230572	-2.560749
H42	11.305817	5.850743	-2.344612
H43	12.538025	4.716869	-1.792484
C44	14.748623	8.365404	1.669412
H45	15.496009	8.422403	0.871542
H46	15.199113	7.785323	2.091216
H47	14.563800	9.397839	2.005729
C48	13.343948	4.926426	3.552852
H49	12.944188	5.356843	2.624567
C50	14.606742	2.942363	6.947083
H51	15.549164	2.373916	6.881672
C52	14.765388	4.053676	7.959400
H53	15.578454	4.728846	7.672876
H54	14.982639	3.630549	8.946739
H55	13.834939	4.633943	8.027945
C56	13.437422	2.032371	7.264390



H57	13.320217	1.236030	6.521634	H62	10.802740	0.869521	5.262572
H58	12.515029	2.626155	7.279059	H63	11.764442	-0.518083	5.820857
H59	13.580071	1.566350	8.246339	C64	13.530700	2.521627	3.679492
C60	14.437230	2.907926	4.519731	C65	14.206402	1.432887	3.128824
C61	14.971299	1.631822	4.371073	H66	14.191361	0.464753	3.621437
H62	15.373485	1.094543	5.225376	C67	14.907142	1.585291	1.935880
C63	14.993488	1.041169	3.110510	H68	15.435658	0.729527	1.520753
H64	15.414841	0.043672	3.003431	C69	14.926852	2.805691	1.272572
C65	14.487121	1.704837	1.997331	H70	15.466404	2.915218	0.334946
H66	14.508318	1.230922	1.019200	C71	14.227249	3.880165	1.808166
C67	13.951037	2.974678	2.152112	H72	14.187216	4.835449	1.281106
H68	13.543892	3.516794	1.297729	C73	13.551334	3.770356	3.025596
C69	13.910754	3.600809	3.404823	74			
C70	11.775221	9.738979	4.839004	3a Na+ - P dis			
C71	11.931795	9.505949	3.514980	Na80	14.756246	8.680758	3.845895
H72	11.422213	10.633204	5.342217	Ru9	13.258396	5.752982	5.213445
H73	11.741343	10.162465	2.672608	C110	11.577018	5.270966	6.771250
Na80	14.521410	9.056460	4.639484	C111	15.575119	6.330990	4.605349
74				O12	11.426170	2.992123	2.135648
3a Na+ - TS dis				N13	12.647564	8.745008	5.459498
Na80	15.000631	8.687195	4.284610	N14	12.225856	8.064184	3.308739
N1	12.662220	8.709657	5.532544	B15	12.551723	7.513239	4.642278
N2	12.554252	8.263159	3.289732	C16	12.696156	8.877080	6.886732
B3	12.645000	7.568733	4.590458	C17	11.495855	8.784146	7.608905
C4	12.469181	8.716816	6.952971	C18	11.541992	8.910845	8.993768
C5	11.156501	8.689506	7.449362	H19	10.612702	8.829969	9.559500
C6	10.969498	8.708344	8.827799	C20	12.736110	9.132336	9.675276
H7	9.951955	8.679166	9.220398	C21	13.904375	9.259408	8.930725
C8	12.040379	8.754357	9.717628	H22	14.845366	9.462868	9.444034
C9	13.328609	8.810010	9.195547	C23	13.905309	9.140014	7.541290
H10	14.179081	8.871945	9.876161	C24	10.192779	8.536590	6.914626
C11	13.562863	8.796792	7.820831	H25	9.352885	8.684792	7.600924
C12	9.981370	8.611359	6.525264	H26	10.155050	7.500393	6.551460
H13	9.045240	8.764323	7.071834	H27	10.052384	9.200320	6.051797
H14	9.944171	7.616833	6.059712	C28	12.757450	9.221627	11.171945
H15	10.034657	9.356356	5.720998	H29	13.627615	9.781347	11.531814
C16	11.804346	8.732903	11.198338	H30	12.801875	8.222667	11.623740
H17	12.651896	9.154818	11.749361	H31	11.855052	9.708791	11.558610
H18	11.658708	7.706425	11.557813	C32	15.188676	9.324898	6.785568
H19	10.905764	9.298606	11.470161	H33	15.993574	9.642645	7.455918
C20	14.970036	8.898119	7.307963	H34	15.091057	10.113994	6.021965
H21	15.675969	9.044426	8.131581	H35	15.519956	8.390405	6.309508
H22	15.088481	9.769118	6.641363	C36	11.732766	7.415300	2.134241
H23	15.282994	7.986685	6.777266	C37	10.370526	7.079864	2.078302
C24	12.246583	7.737134	1.999041	C38	9.875434	6.501981	0.912565
C25	10.915456	7.393197	1.718379	H39	8.814022	6.251211	0.859577
C26	10.614106	6.876556	0.461091	C40	10.695855	6.235177	-0.184488
H27	9.582354	6.600478	0.238111	C41	12.047874	6.551424	-0.086880
C28	11.592966	6.697233	-0.514881	H42	12.709008	6.334954	-0.927622
C29	12.902369	7.062235	-0.211586	C43	12.581542	7.145650	1.057052
H30	13.680737	6.935581	-0.965933	C44	9.486395	7.296936	3.268187
C31	13.248322	7.580181	1.036316	H45	8.445441	7.051502	3.035391
C32	9.854723	7.529428	2.768391	H46	9.523850	8.334487	3.624960
H33	8.863578	7.319454	2.354156	H47	9.804647	6.662314	4.108169
H34	9.838306	8.536006	3.205903	C48	10.123899	5.639253	-1.437601
H35	10.029431	6.828487	3.597976	H49	9.472593	6.354169	-1.956443
C36	11.242566	6.105313	-1.847362	H50	9.514333	4.751615	-1.221139
H37	11.957651	6.401635	-2.622206	H51	10.911640	5.340225	-2.138308
H38	10.242080	6.412718	-2.171865	C52	14.046503	7.458277	1.128877
H39	11.244258	5.008925	-1.803403	H53	14.555017	7.187444	0.198392
C40	14.676902	7.927330	1.338338	H54	14.531633	6.894318	1.940366
H41	15.309299	7.799606	0.453711	H55	14.218347	8.536943	1.276167
H42	15.084340	7.269786	2.123229	C56	12.747173	4.759542	3.765204
H43	14.779435	8.979096	1.650505	H57	12.013429	5.107978	3.028283
C44	12.501372	9.909989	4.823759	C58	10.741000	2.240462	1.134605
C45	12.433539	9.647682	3.498884	H59	10.691864	1.183868	1.443431
H46	12.278317	10.326829	2.667430	C60	9.337692	2.802777	1.098249
H47	12.413850	10.858221	5.343695	H61	8.831117	2.643923	2.055316
Ru48	13.174015	5.704984	5.065722	H62	8.750160	2.326840	0.304678
C149	11.296109	5.302999	6.422765	H63	9.381247	3.883129	0.913717
C150	15.572535	6.198844	4.756392	C64	11.466417	2.376718	-0.190298
O51	12.869170	2.510990	4.856301	H65	12.474101	1.949145	-0.146567
C52	12.751690	4.910011	3.494080	H66	11.561295	3.441836	-0.438105
H53	12.053134	5.340383	2.760620	H67	10.912964	1.876232	-0.993539
C54	12.852859	1.344437	5.681278	C68	12.547018	2.506577	2.715556
H55	13.846931	0.868089	5.640713	C69	13.033589	1.213802	2.519271
C56	12.586510	1.841212	7.084556	H70	12.541027	0.531720	1.832549
H57	13.383773	2.514573	7.416592	C71	14.156143	0.779247	3.215473
H58	12.517508	0.998703	7.782440	H72	14.518284	-0.234065	3.053738
H59	11.648393	2.408497	7.106632	C73	14.813391	1.622383	4.104033
C60	11.783432	0.383636	5.197572	H74	15.692994	1.280214	4.642847
H61	11.945052	0.079401	4.157558	C75	14.346847	2.914844	4.279123

H76	14.881466	3.596291	4.940519
C77	13.217341	3.395414	3.595050
C78	12.311512	9.857272	4.675635
C79	12.061536	9.458616	3.407452
H80	12.252494	10.850637	5.108449
H81	11.742939	10.043652	2.551446
80			
3b	Na+ - S		
Ru1	13.127709	5.702199	5.240178
C12	11.456652	5.105453	6.807190
C13	15.351549	6.541467	4.545804
O4	14.295492	3.568282	5.714743
N5	12.173177	8.612046	5.570542
N6	11.788035	7.955716	3.415487
B7	12.205888	7.401356	4.715562
C8	12.172211	8.634703	7.003383
C9	10.959417	8.417394	7.678302
C10	10.964999	8.383503	9.069116
H11	10.025954	8.201091	9.594102
C12	12.135785	8.545389	9.806232
C13	13.316679	8.795742	9.115067
H14	14.239274	8.957471	9.675060
C15	13.354514	8.853191	7.721374
C16	9.690278	8.163132	6.926055
H17	8.822756	8.225903	7.591076
H18	9.718711	7.150016	6.502022
H19	9.540562	8.864609	6.095394
C20	12.120669	8.435344	11.301884
H21	12.972229	8.954907	11.754784
H22	12.172322	7.385598	11.618601
H23	11.201113	8.853410	11.727348
C24	14.652227	9.164910	7.035232
H25	15.413165	9.469279	7.761203
H26	14.539967	10.006666	6.331943
H27	15.055003	8.297319	6.492193
C28	11.404761	7.229667	2.248362
C29	10.145121	6.609902	2.224250
C30	9.783456	5.873286	1.099024
H31	8.807777	5.384822	1.079959
C32	10.637606	5.731752	0.006540
C33	11.879187	6.360591	0.055002
H34	12.562519	6.259144	-0.789685
C35	12.279687	7.106076	1.163012
C36	9.238920	6.680604	3.415121
H37	8.252748	6.265007	3.184259
H38	9.105027	7.709356	3.774062
H39	9.660481	6.107549	4.254555
C40	10.238351	4.895265	-1.172919
H41	10.783020	5.185558	-2.077761
H42	9.165421	4.978526	-1.379853
H43	10.448735	3.832992	-0.992919
C44	13.652909	7.708626	1.201457
H45	14.162942	7.593581	0.239592
H46	14.275629	7.206797	1.959180
H47	13.618580	8.789256	1.414279
C48	12.699548	4.662661	3.801441
H49	12.049004	4.987282	2.977786
C50	14.855458	3.078284	6.946487
H51	15.735087	2.461898	6.697479
C52	15.306820	4.305292	7.706050
H53	16.009110	4.896327	7.108866
H54	15.794779	4.006753	8.640957
H55	14.439813	4.933819	7.952319
C56	13.819095	2.274999	7.705852
H57	13.490499	1.392151	7.146970
H58	12.942963	2.908130	7.893562
H59	14.231783	1.939383	8.664494
C60	14.002763	2.735093	4.692146
C61	14.463528	1.427485	4.577045
H62	15.084305	0.986697	5.352063
C63	14.128235	0.679975	3.451364
H64	14.495504	-0.340943	3.368202
C65	13.336057	1.218155	2.442016
H66	13.079937	0.622635	1.569272
C67	12.873276	2.520088	2.565494
H68	12.248103	2.965854	1.790964
C69	13.189803	3.303203	3.683414
C70	11.672118	9.714495	4.835155
C71	11.438689	9.323388	3.553384
C72	11.456360	11.040623	5.476068
H73	11.182367	11.795441	4.732043
H74	10.655273	11.005549	6.227095

H75	12.353283	11.394323	6.003468
C76	10.873770	10.096105	2.414283
H77	10.736305	11.147269	2.686528
H78	11.512394	10.058293	1.520725
H79	9.895242	9.701037	2.107700
Na80	14.236025	8.818655	4.000957
80			
3b	Na+ - TS dis		
Na80	14.862392	8.665764	4.220493
N1	12.592298	8.706131	5.507858
N2	12.386825	8.275494	3.273064
B3	12.527546	7.575892	4.559419
C4	12.433291	8.660242	6.931458
C5	11.133051	8.600087	7.458555
C6	10.975173	8.560191	8.840036
H7	9.966400	8.506980	9.252564
C8	12.065177	8.573753	9.707242
C9	13.340765	8.660253	9.159181
H10	14.205969	8.697283	9.823146
C11	13.544977	8.710159	7.780177
C12	9.936146	8.543488	6.560062
H13	9.015688	8.729252	7.123348
H14	9.863877	7.542497	6.112164
H15	9.990802	9.270411	5.739018
C16	11.863062	8.485568	11.190449
H17	12.712108	8.906121	11.740438
H18	11.751258	7.441765	11.509878
H19	10.956941	9.016185	11.504637
C20	14.941918	8.841453	7.246244
H21	15.658570	8.985872	8.061153
H22	15.039721	9.722678	6.589262
H23	15.259836	7.943119	6.696611
C24	12.063163	7.720417	1.999979
C25	10.733404	7.349097	1.746783
C26	10.418972	6.794192	0.508628
H27	9.387736	6.497473	0.310309
C28	11.385082	6.597751	-0.476553
C29	12.694476	6.985193	-0.201817
H30	13.464472	6.842160	-0.962198
C31	13.052077	7.541201	1.026405
C32	9.687831	7.489962	2.811321
H33	8.690633	7.275569	2.413627
H34	9.675402	8.496754	3.249186
H35	9.878733	6.791815	3.639969
C36	11.024435	5.960158	-1.785125
H37	11.719246	6.249061	-2.581183
H38	10.011621	6.235524	-2.100232
H39	11.052113	4.865747	-1.709444
C40	14.485335	7.893487	1.299491
H41	15.100900	7.765218	0.402843
H42	14.908927	7.236480	2.076583
H43	14.595617	8.945639	1.609566
C44	12.386779	9.928720	4.818076
C45	12.260912	9.672619	3.488614
Ru46	13.066380	5.704091	5.024494
C147	11.192661	5.253165	6.375688
C148	15.463735	6.184567	4.684811
O49	12.885210	2.504521	4.870750
C50	12.658648	4.887792	3.457675
H51	11.957388	5.312449	2.723478
C52	12.906738	1.344560	5.704232
H53	13.911125	0.890454	5.654985
C54	12.647010	1.848269	7.106638
H55	13.433285	2.542511	7.422190
H56	12.605801	1.010891	7.813110
H57	11.696187	2.394166	7.134638
C58	11.852060	0.355257	5.244880
H59	12.003236	0.046370	4.204575
H60	10.861202	0.818437	5.323012
H61	11.864947	-0.541867	5.875241
C62	13.500636	2.514330	3.669453
C63	14.189817	1.434027	3.117934
H64	14.227354	0.479747	3.636037
C65	14.836081	1.575480	1.893546
H66	15.375717	0.725914	1.479374
C67	14.786352	2.777212	1.198210
H68	15.281685	2.878653	0.235370
C69	14.074307	3.842235	1.736049
H70	13.982573	4.781582	1.186933
C71	13.454072	3.746986	2.984865
C72	12.297608	11.224496	5.545296
H73	12.255071	12.063459	4.843327

H74	11.402220	11.273841	6.180082
H75	13.154717	11.384612	6.213931
C76	11.981943	10.608218	2.365756
H77	11.994057	11.646079	2.713148
H78	12.710456	10.516449	1.548292
H79	10.995928	10.418321	1.919392
80			
3b	Na+	-	P dis
Na80	14.622547	8.910337	3.913095
Ru9	13.378945	5.797104	5.039779
Cl10	11.728744	5.099705	6.553386
Cl11	15.641052	6.590421	4.465429
O12	11.880498	2.904054	1.883213
N13	12.517666	8.701933	5.466840
N14	12.168722	8.136977	3.276414
B15	12.527628	7.530492	4.568078
C16	12.523222	8.694527	6.900001
C17	11.316132	8.451797	7.575168
C18	11.322792	8.425622	8.966014
H19	10.387723	8.227115	9.492217
C20	12.487389	8.630813	9.701871
C21	13.662389	8.904219	9.009230
H22	14.579606	9.095061	9.568601
C23	13.700073	8.945869	7.615486
C24	10.047362	8.188978	6.824686
H25	9.179291	8.265827	7.487626
H26	10.069722	7.170472	6.412935
H27	9.903460	8.882611	5.986190
C28	12.470516	8.544729	11.198791
H29	13.302374	9.099587	11.646194
H30	12.555788	7.502611	11.531748
H31	11.535555	8.938548	11.613710
C32	14.990570	9.278438	6.924504
H33	15.751982	9.585391	7.648775
H34	14.867500	10.124131	6.227025
H35	15.398144	8.415564	6.377840
C36	11.752975	7.479916	2.079529
C37	10.443350	6.987215	2.005112
C38	10.018143	6.393609	0.817001
H39	8.993451	6.023691	0.751620
C40	10.861719	6.261260	-0.282456
C41	12.171785	6.726719	-0.167248
H42	12.853085	6.616211	-1.013270
C43	12.631650	7.338397	0.996560
C44	9.534774	7.056142	3.194170
H45	8.521059	6.734509	2.935089
H46	9.478344	8.068288	3.615968
H47	9.902911	6.401509	3.997874
C48	10.382507	5.644327	-1.564092
H49	10.516651	6.328857	-2.410735
H50	9.320487	5.380994	-1.511449
H51	10.937477	4.727084	-1.804567
C52	14.054010	7.806717	1.090515
H53	14.584581	7.651077	0.145806
H54	14.601198	7.249337	1.866848
H55	14.111912	8.886115	1.309121
C56	12.981232	4.789805	3.565657
H57	12.253750	5.086970	2.800238
C58	11.389295	2.152988	0.773808
H59	11.378289	1.081396	1.031068
C60	9.965827	2.619234	0.569125
H61	9.355143	2.395085	1.449293
H62	9.520617	2.129427	-0.304423
H63	9.954429	3.704592	0.414068
C64	12.268759	2.401097	-0.436907
H65	13.288820	2.032904	-0.282253
H66	12.325659	3.482555	-0.619062
H67	11.856963	1.913067	-1.328119
C68	13.001420	2.513470	2.533336
C69	13.587843	1.255707	2.387560
H70	13.178931	0.530116	1.690433
C71	14.698659	0.911576	3.148770
H72	15.138656	-0.075905	3.025359
C73	15.244725	1.812464	4.055845
H74	16.115781	1.542525	4.646882
C75	14.677708	3.069454	4.183765
H76	15.127437	3.794517	4.862387
C77	13.555564	3.460291	3.431651
C78	12.074765	9.847596	4.760462
C79	11.864872	9.514021	3.458551
C86	11.871121	11.150843	5.449651
H87	11.638134	11.942106	4.730151

H88	11.044484	11.101216	6.171420
H89	12.756629	11.461138	6.021151
C89	11.358212	10.349812	2.336415
H90	11.270732	11.397276	2.641648
H91	12.011300	10.307713	1.453612
H92	10.366566	10.017179	1.999767
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3c	Na+	-	S
Ru1	13.145685	5.698697	5.230509
Cl2	11.182198	4.780744	6.177554
Cl3	15.386708	6.734547	5.308601
O	14.309062	3.551409	5.713769
N5	11.929234	8.484829	5.653799
N6	12.179260	8.108363	3.388948
B7	12.278117	7.403567	4.689769
C10	11.590226	8.332662	7.037465
C11	10.282622	7.941724	7.368833
C12	9.966209	7.753452	8.710245
H13	8.955333	7.437535	8.971892
C14	10.903053	7.945373	9.723727
C15	12.177323	8.376112	9.369001
H16	12.914326	8.567809	10.150573
C17	12.536753	8.583052	8.037052
C18	9.254579	7.711320	6.304896
H19	8.269950	7.532609	6.748960
H20	9.520270	6.825639	5.712150
H21	9.171094	8.566556	5.621550
C22	10.544337	7.687744	11.156780
H23	11.196284	8.240068	11.842387
H24	10.641414	6.622227	11.400486
H25	9.507462	7.972168	11.369272
C26	13.908658	9.099803	7.713414
H27	14.438081	9.396631	8.624564
H28	13.850805	10.001420	7.080908
H29	14.528871	8.339539	7.216375
C30	12.187347	7.548718	2.076433
C31	11.035140	6.888037	1.623319
C32	11.056647	6.308742	0.357436
H33	10.167829	5.784703	0.002386
C34	12.183563	6.371598	-0.461566
C35	13.305249	7.050907	0.007892
H36	14.193815	7.115322	-0.622004
C37	13.326131	7.642827	1.270134
C38	9.835123	6.757912	2.510447
H39	8.992405	6.316677	1.968843
H40	9.515442	7.729243	2.909567
H41	10.056926	6.113182	3.373894
C42	12.189464	5.698776	-1.802512
H43	12.939409	6.135216	-2.470766
H44	11.212207	5.773288	-2.292857
H45	12.419739	4.629310	-1.708033
C46	14.567642	8.325078	1.765116
H47	15.319828	8.402129	0.973359
H48	15.024691	7.753151	2.588793
H49	14.352016	9.352639	2.099427
C50	13.196145	4.867272	3.604532
H51	12.775805	5.291978	2.683346
C52	14.564712	2.904775	6.974769
H53	15.511772	2.347898	6.882598
C54	14.740182	4.022006	7.977813
H55	15.537667	4.704589	7.666454
H56	14.989012	3.605374	8.960429
H57	13.806213	4.593237	8.070283
C58	13.417097	1.981783	7.330852
H59	13.285624	1.182144	6.594076
H60	12.488373	2.564056	7.373094
H61	13.596495	1.520246	8.308879
C62	14.328210	2.860861	4.552803
C63	14.866195	1.587336	4.394369
H64	15.289475	1.053480	5.240506
C65	14.864374	0.994725	3.134560
H66	15.288270	-0.000877	3.020454
C67	14.331030	1.653492	2.031006
H68	14.333695	1.177739	1.053572
C69	13.791419	2.920449	2.195143
H70	13.362996	3.458662	1.348840
C71	13.773611	3.548171	3.447963
C72	11.558534	9.643118	4.962221
C73	11.706781	9.413468	3.581508
C74	11.414618	10.408301	2.657347
C75	10.974544	11.643606	3.138464
C76	10.831695	11.872721	4.505493

C77	11.122548	10.873704	5.437205
H80	11.511083	10.212952	1.590328
H81	10.732528	12.434541	2.432357
H82	10.479395	12.840463	4.855039
H83	10.990335	11.032054	6.506643
Na80	14.344903	9.042791	4.720970
80			
3c Na+ - TS dis			
Na80	14.856176	8.575380	4.241735
N1	12.526247	8.669578	5.501251
N2	12.329430	8.242269	3.237741
B3	12.425234	7.543095	4.538441
C4	12.366848	8.640064	6.925740
C5	11.064994	8.626698	7.451031
C6	10.908446	8.598539	8.832709
H7	9.899288	8.578423	9.246664
C8	11.999816	8.591206	9.699010
C9	13.276880	8.645418	9.150276
H10	14.143033	8.672297	9.813139
C11	13.480801	8.677127	7.770834
C12	9.870357	8.631253	6.548728
H13	8.948797	8.758465	7.125528
H14	9.802594	7.675065	6.012493
H15	9.920425	9.437079	5.804656
C16	11.796595	8.521460	11.182884
H17	12.664643	8.907055	11.728492
H18	11.638153	7.485877	11.509014
H19	10.915959	9.094524	11.494945
C20	14.877481	8.786758	7.231273
H21	15.598761	8.930788	8.041985
H22	14.977021	9.664216	6.570080
H23	15.182697	7.877835	6.691908
C24	12.020395	7.722044	1.945776
C25	10.682257	7.426283	1.644624
C26	10.382842	6.915385	0.384366
H27	9.345629	6.675424	0.145816
C28	11.369783	6.700139	-0.576549
C29	12.686045	7.023019	-0.255073
H30	13.470747	6.871465	-0.998315
C31	13.030249	7.531957	0.997090
C32	9.612048	7.615665	2.676209
H33	8.621904	7.412805	2.256218
H34	9.610918	8.637918	3.076634
H35	9.761946	6.938797	3.530210
C36	11.020782	6.118493	-1.913908
H37	11.756022	6.392729	-2.678037
H38	10.035121	6.456166	-2.253172
H39	10.988750	5.022578	-1.870087
C40	14.463685	7.839350	1.318468
H41	15.102217	7.710224	0.438366
H42	14.847114	7.159143	2.096320
H43	14.583112	8.885290	1.644869
C44	12.384450	9.886470	4.821939
C45	12.260883	9.627156	3.445490
C46	12.116000	10.664856	2.533386
C47	12.100130	11.972189	3.024177
C48	12.224264	12.229615	4.388133
C49	12.367986	11.188225	5.307205
H50	11.999933	10.452347	1.471697
H51	11.980337	12.800200	2.329381
H52	12.199602	13.256220	4.746180
H53	12.440050	11.375261	6.377603
Ru54	12.870937	5.667709	5.010440
C155	10.963088	5.287629	6.332762
C156	15.287760	6.056661	4.714635
O57	12.556647	2.522324	4.821806
C58	12.445823	4.893359	3.427849
H59	11.764746	5.348257	2.693247
C60	12.450516	1.344565	5.624536
H61	13.407336	0.797479	5.580416
C62	12.212967	1.833609	7.035438
H63	13.052907	2.445248	7.381630
H64	12.085577	0.985129	7.717489
H65	11.314423	2.461392	7.064723
C66	11.314599	0.476691	5.117601
H67	11.460902	0.177131	4.073887
H68	10.374479	1.037241	5.184045
H69	11.220402	-0.430436	5.725882
C70	13.178080	2.496619	3.623592
C71	13.805756	1.382825	3.066626
H72	13.776508	0.420575	3.569977
C73	14.479627	1.504087	1.854810

H74	14.972385	0.629496	1.434906
C75	14.518551	2.717270	1.178847
H76	15.037129	2.801448	0.226876
C77	13.861828	3.816126	1.718792
H78	13.831938	4.765476	1.180488
C79	13.215523	3.737337	2.954887
80			
3c Na+ - P dis			
Na80	14.618690	8.764525	3.833894
Ru9	13.237160	5.764880	5.228999
C110	11.640141	5.167920	6.833139
C111	15.510957	6.430316	4.560595
O12	11.468507	2.948431	2.149074
N13	12.548871	8.716565	5.519179
N14	12.048307	8.024880	3.365111
B15	12.449831	7.488608	4.688465
C16	12.655339	8.831694	6.944123
C17	11.492087	8.676545	7.715629
C18	11.591431	8.806406	9.097293
H19	10.692642	8.679892	9.702555
C20	12.800458	9.095753	9.726720
C21	13.927603	9.284838	8.933560
H22	14.876689	9.542604	9.405985
C23	13.875225	9.164006	7.545194
C24	10.174363	8.380146	7.070734
H25	9.360659	8.453945	7.799158
H26	10.172965	7.359307	6.665325
H27	9.959249	9.073960	6.247718
C28	12.879472	9.197142	11.220579
H29	13.747258	9.784171	11.540343
H30	12.969514	8.203715	11.677542
H31	11.980100	9.662854	11.639582
C32	15.110166	9.425882	6.733428
H33	15.923571	9.792728	7.367580
H34	14.928318	10.208953	5.978901
H35	15.475981	8.511777	6.243400
C36	11.572357	7.354012	2.196356
C37	10.221472	6.974878	2.145020
C38	9.741422	6.381096	0.980897
H39	8.688418	6.096590	0.931484
C40	10.565265	6.144275	-0.120875
C41	11.905412	6.509275	-0.030221
H42	12.568652	6.321747	-0.876264
C43	12.422993	7.121822	1.111494
C44	9.333136	7.182374	3.333265
H45	8.308586	6.861693	3.120147
H46	9.304377	8.236282	3.640609
H47	9.696360	6.607099	4.196924
C48	10.008372	5.534357	-1.374183
H49	9.335086	6.231290	-1.889435
H50	9.425821	4.628402	-1.159520
H51	10.802990	5.261292	-2.077782
C52	13.871330	7.506334	1.167718
H53	14.380995	7.267305	0.229106
H54	14.395757	6.963521	1.968958
H55	13.984462	8.593025	1.316064
C56	12.726844	4.751398	3.792594
H57	11.958154	5.070509	3.079024
C58	10.798637	2.167487	1.158990
H59	10.795539	1.111014	1.471753
C60	9.373979	2.674110	1.141166
H61	8.884946	2.492753	2.103341
H62	8.796349	2.177853	0.352773
H63	9.372966	3.755740	0.959824
C64	11.500281	2.327421	-0.176192
H65	12.524464	1.939807	-0.144972
H66	11.549962	3.394317	-0.429220
H67	10.956078	1.802496	-0.970167
C68	12.608989	2.503075	2.721307
C69	13.144798	1.231485	2.513150
H70	12.675678	0.535729	1.823825
C71	14.287234	0.835993	3.199751
H72	14.687050	-0.161478	3.028480
C73	14.917153	1.697463	4.090913
H74	15.812349	1.385663	4.622315
C75	14.401285	2.968791	4.278581
H76	14.911912	3.664279	4.944459
C77	13.249306	3.410161	3.605021
C87	11.834008	9.408100	3.465255
C88	12.140328	9.827305	4.773075
C89	12.037755	11.163859	5.140941
C90	11.619862	12.079117	4.172555

C91 11.316581 11.665571 2.876769  
 C92 11.419678 10.322831 2.505133  
 H95 12.256654 11.469775 6.162814  
 H96 11.523214 13.129262 4.438426  
 H97 10.986601 12.396737 2.142436  
 H98 11.166254 9.988831 1.500069  
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 Ru1 12.882021 5.701526 5.250548  
 C12 10.845170 4.884684 6.219505  
 C13 15.097958 6.577164 5.001478  
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 N5 11.840673 8.505405 5.530304  
 N6 11.428112 7.978698 3.536066  
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 C10 11.967009 7.728430 9.136320  
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 C12 13.292793 8.040786 9.438651  
 C13 14.098223 8.600919 8.447739  
 H14 15.118015 8.901473 8.689376  
 C15 13.632296 8.799806 7.150710  
 C16 9.985913 7.709276 7.585958  
 H17 9.559523 6.970026 8.270319  
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 H19 9.453935 8.659016 7.736020  
 C20 13.841338 7.776363 10.808228  
 H21 14.662504 8.458198 11.053274  
 H22 14.236475 6.753864 10.876070  
 H23 13.068947 7.875857 11.578532  
 C24 14.456286 9.538632 6.142227  
 H25 15.523377 9.414646 6.347695  
 H26 14.221361 10.610854 6.191229  
 H27 14.279660 9.196711 5.118879  
 C28 11.387345 7.225432 2.329146  
 C29 10.257522 6.442303 2.071922  
 C30 10.240251 5.712391 0.886778  
 H31 9.376958 5.083394 0.665628  
 C32 11.297492 5.769404 -0.023334  
 C33 12.393308 6.582389 0.265132  
 H34 13.220702 6.638385 -0.443173  
 C35 12.458092 7.332460 1.438400  
 C36 9.131899 6.378107 3.056219  
 H37 8.315339 5.757531 2.674758  
 H38 8.733595 7.380843 3.256732  
 H39 9.464565 5.952450 4.014788  
 C40 11.235447 4.988831 -1.302764  
 H41 12.228736 4.858822 -1.745095  
 H42 10.610141 5.500639 -2.045503  
 H43 10.797526 3.996141 -1.146327  
 C44 13.639577 8.193755 1.758575  
 H45 14.334314 8.232078 0.914041  
 H46 14.187206 7.809757 2.632638  
 H47 13.325021 9.219915 1.988044  
 C48 12.838268 4.736251 3.695332  
 H49 12.399666 5.094654 2.759273  
 C50 14.184352 3.476573 7.297021  
 H51 15.169356 2.989097 7.242258  
 C52 14.310310 4.762173 8.078871  
 H53 15.019848 5.447952 7.602968  
 H54 14.665319 4.527017 9.089396  
 H55 13.334892 5.261620 8.171956  
 C56 13.127550 2.545961 7.850295  
 H57 13.036260 1.625665 7.263875  
 H58 12.156448 3.054272 7.842410  
 H59 13.382291 2.271312 8.880387  
 C60 13.971107 2.953542 4.906928  
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 H62 14.991416 1.334558 5.917441  
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 H72 11.047084 10.466029 5.617039  
 O73 10.365431 9.912644 2.750368  
 73

4a - S - cis  
 Ru1 12.894423 5.700453 5.368826  
 C12 10.736652 5.021860 5.981319  
 C13 13.822483 4.127269 6.838432  
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 N6 11.216281 7.819638 3.637118  
 N7 11.961256 7.552104 4.730874  
 C8 12.146207 8.449577 6.934540  
 C9 11.477802 7.951540 8.056409  
 C10 12.168647 8.004453 9.269103  
 H11 11.680715 7.602374 10.157522  
 C12 13.437763 8.560292 9.380182  
 C13 14.025173 9.123943 8.244367  
 H14 14.998356 9.609684 8.327519  
 C15 13.395871 9.086617 7.007867  
 C16 10.071556 7.437521 8.042418  
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 C24 14.000006 9.745452 5.803706  
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 H26 13.295154 10.447408 5.338227  
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 C32 11.892218 6.048034 -0.108643  
 C33 12.804428 6.960362 0.416242  
 H34 13.703720 7.206212 -0.150410  
 C35 12.606316 7.557496 1.657542  
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 H37 8.681706 5.211470 2.150981  
 H38 8.622423 6.900600 2.703420  
 H39 9.482334 5.687944 3.668849  
 C40 12.129076 5.397252 -1.438599  
 H41 13.154215 5.558641 -1.789288  
 H42 11.448583 5.791758 -2.203668  
 H43 11.955123 4.314749 -1.385672  
 C44 13.601818 8.533560 2.204694  
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 H51 17.000500 6.793771 4.421735  
 C52 16.127196 6.901159 6.369489  
 H53 15.702938 7.893973 6.198375  
 H54 17.083485 7.024582 6.890681  
 H55 15.452387 6.324826 7.014763  
 C56 16.979139 4.805291 5.290948  
 H57 17.184810 4.279703 4.353648  
 H58 16.299876 4.194776 5.896876  
 H59 17.927394 4.919524 5.828368  
 C60 15.059046 5.430310 3.177217  
 C61 16.107941 5.476778 2.267049  
 H62 17.016708 6.029150 2.488313  
 C63 15.994648 4.782813 1.064345  
 H64 16.823085 4.812894 0.359854  
 C65 14.850763 4.049749 0.759500  
 H66 14.783732 3.501438 -0.177057  
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 H68 12.877452 3.491430 1.433987  
 C69 13.877444 4.731375 2.870844  
 C70 10.550827 9.221465 5.193802  
 C71 10.274984 8.876414 3.837962  
 H72 10.128393 9.989303 5.824085  
 O73 9.510345 9.292461 2.985219  
 85  
 4a - TS inter  
 C80 14.442916 3.778596 7.596930  
 C81 13.563324 4.395492 8.423297  
 H82 13.744005 5.459907 8.611726  
 C83 12.451404 3.773963 9.196337  
 H84 12.596799 3.945813 10.270797  
 H85 11.489846 4.224884 8.915406

H86	12.374838	2.694508	9.035020	C2	14.187504	4.535040	7.075607
C87	14.523198	2.320222	7.297276	H3	15.175066	4.938455	6.847064
H88	13.625627	1.767103	7.589046	C4	13.631371	4.914927	8.412027
H89	14.696188	2.146027	6.228084	H5	13.575132	6.008987	8.517525
H90	15.380801	1.882223	7.826610	H6	12.633401	4.509413	8.593751
H91	15.242946	4.399344	7.189517	H7	14.315444	4.564062	9.198409
N1	11.501495	8.330531	5.550830	Ru9	12.933115	5.597066	5.535803
N2	11.228439	7.190125	3.786002	C110	10.763914	5.161962	6.560368
N3	11.990587	7.275960	4.907647	C111	15.111150	6.348390	4.756865
C4	12.111257	8.797447	6.771781	O12	10.943129	2.713305	2.774381
C5	11.513732	8.511301	8.002548	N13	11.971606	8.587229	5.477104
C6	12.196172	8.934333	9.144602	N14	11.982359	7.965986	3.468915
H7	11.762907	8.708163	10.119796	N15	12.137702	7.512918	4.729450
C8	13.385504	9.652022	9.072827	C16	12.127267	8.521381	6.905379
C9	13.885462	9.995307	7.816984	C17	10.990997	8.286165	7.686313
H10	14.797910	10.587826	7.746033	C18	11.179299	8.199005	9.062341
C11	13.270936	9.575027	6.645470	H19	10.318618	7.985642	9.696435
C12	10.166277	7.871975	8.147096	C20	12.433653	8.377069	9.645388
H13	10.166819	7.154513	8.975862	C21	13.517210	8.700172	8.829095
H14	9.848011	7.330670	7.254556	H22	14.491088	8.893232	9.280393
H15	9.416298	8.640232	8.378259	C23	13.390694	8.793972	7.443855
C16	14.122866	10.050352	10.314992	C24	9.624011	8.207168	7.081918
H17	14.545110	11.057595	10.226384	H25	8.927046	7.719358	7.769396
H18	14.960451	9.366227	10.500952	H26	9.621575	7.633755	6.150476
H19	13.474665	10.026091	11.196989	H27	9.244553	9.215906	6.868320
C20	13.849627	9.929868	5.311638	C28	12.618430	8.202395	11.122465
H21	14.483216	10.818502	5.393371	H29	13.452052	8.803916	11.500534
H22	13.075722	10.128986	4.560211	H30	12.839371	7.152862	11.360122
H23	14.473573	9.102147	4.950695	H31	11.715317	8.476349	11.678432
C24	11.550315	6.302849	2.714441	C32	14.533341	9.260039	6.595140
C25	10.663840	5.262470	2.400654	H33	15.481762	9.151317	7.130163
C26	11.025324	4.401298	1.366982	H34	14.409411	10.322717	6.347180
H27	10.356154	3.576683	1.115399	H35	14.618592	8.702384	5.656134
C28	12.193617	4.580205	0.628343	C36	12.056875	7.111639	2.330820
C29	12.998304	5.681896	0.913041	C37	10.949244	6.323193	2.001018
H30	13.888625	5.865195	0.309143	C38	11.049102	5.515176	0.871548
C31	12.691461	6.565321	1.945027	H39	10.198827	4.892168	0.593022
C32	9.342310	5.128208	3.085793	C40	12.198861	5.493356	0.084012
H33	8.833122	4.210968	2.771679	C41	13.253319	6.343667	0.413908
H34	8.709878	5.986213	2.822667	H42	14.141020	6.366731	-0.219759
H35	9.450654	5.121002	4.176970	C43	13.198743	7.183624	1.522600
C36	12.571756	3.603975	-0.443474	C44	9.690712	6.366828	2.814367
H37	13.277394	4.039932	-1.158922	H45	8.924673	5.720094	2.372210
H38	11.693826	3.253809	-0.998262	H46	9.290567	7.389052	2.855896
H39	13.053260	2.719753	-0.002085	H47	9.843948	6.041383	3.853829
C40	13.552664	7.763751	2.206594	C48	12.307522	4.570175	-1.092004
H41	14.250258	7.924808	1.378711	H49	12.896074	5.015002	-1.902435
H42	14.143716	7.662068	3.128214	H50	11.321623	4.305154	-1.491629
H43	12.944096	8.670980	2.317994	H51	12.808987	3.636300	-0.799724
C44	10.494484	8.932990	4.906073	C52	14.286111	8.171355	1.804037
C45	10.250170	8.219630	3.693366	H53	15.142401	8.007080	1.142380
O58	9.484499	8.368797	2.756602	H54	14.635847	8.097640	2.840875
H47	10.043394	9.834781	5.291987	H55	13.909340	9.189421	1.639090
Ru48	12.868269	5.688937	5.981711	C56	12.445495	4.526500	4.087223
C149	10.603817	5.016073	6.417540	H57	11.365304	4.615342	3.925664
C150	14.987222	6.840555	6.327831	C58	10.042517	1.731897	2.245307
O51	12.184041	2.523301	5.268414	H59	10.580461	0.773700	2.164728
C52	13.615405	4.927025	4.480910	C60	8.938258	1.607832	3.270327
H53	14.167396	5.671771	3.889308	H61	9.335337	1.286095	4.237802
C54	11.165009	1.515576	5.432360	H62	8.186670	0.883670	2.937957
H55	11.610551	0.528586	5.236116	H63	8.450078	2.579732	3.410063
C56	10.713968	1.545182	6.873226	C64	9.518159	2.164032	0.890480
H57	11.529183	1.266069	7.550081	H65	10.326286	2.356455	0.175048
H58	9.899399	0.824676	7.011489	H66	8.931198	3.085094	1.000050
H59	10.357726	2.545136	7.140619	H67	8.862990	1.392272	0.470490
C60	10.036091	1.804253	4.464931	C68	12.243087	2.723340	2.432219
H61	10.391788	1.840268	3.427617	C69	12.803316	1.884483	1.468098
H62	9.596669	2.778280	4.712353	H70	12.184000	1.194261	0.902844
H63	9.258447	1.035390	4.537020	C71	14.171970	1.930884	1.224118
C64	13.014498	2.451127	4.221479	H72	14.593095	1.269781	0.468565
C65	13.189221	1.298142	3.443079	C73	15.000624	2.800961	1.926702
H66	12.596512	0.410090	3.632153	H74	16.066923	2.833314	1.719463
C67	14.129644	1.260458	2.424254	C75	14.454331	3.625798	2.895574
H68	14.248464	0.341273	1.853505	H76	15.074232	4.334000	3.443246
C69	14.910655	2.374041	2.127060	C77	13.075291	3.618527	3.169514
H70	15.647835	2.343292	1.328959	C78	11.711123	9.705052	4.776742
C71	14.701511	3.532573	2.849221	C79	11.696588	9.363232	3.394378
H72	15.266862	4.431513	2.606580	H80	11.561714	10.653207	5.270942
C73	13.767100	3.614365	3.904739	O80	11.510728	9.973633	2.354896
85				C82	12.684752	2.501066	6.592533
4a - P inter				H83	12.132584	2.185701	5.698697
C1	13.723201	3.522528	6.253134	H84	13.183438	1.611591	7.003715

H85	11.953509	2.863961	7.317581	O12	11.494416	2.530903	2.552436
H86	14.394209	3.243240	5.439046	N13	12.121316	8.577742	5.438592
73				N14	11.774074	8.078699	3.409173
4a - TS dis				N15	12.072369	7.537345	4.612645
N1	11.619985	8.547080	5.563029	C16	12.406263	8.398110	6.838723
N2	11.212890	7.534257	3.741169	C17	11.348838	8.010118	7.672386
N3	12.077830	7.563834	4.788743	C18	11.642390	7.812888	9.015592
C4	12.302344	8.883600	6.787269	H19	10.842608	7.496969	9.685617
C5	11.714657	8.547194	8.012897	C20	12.929709	7.992998	9.521156
C6	12.458775	8.817972	9.160304	C21	13.928318	8.450288	8.665633
H7	12.038154	8.542668	10.127857	H22	14.924571	8.649459	9.061371
C8	13.704639	9.437239	9.106850	C23	13.690229	8.690057	7.312691
C9	14.195706	9.844828	7.867940	C24	9.958603	7.814301	7.153966
H10	15.151678	10.366195	7.814119	H25	9.234018	7.884767	7.970819
C11	13.516048	9.576342	6.686414	H26	9.860970	6.819155	6.703360
C12	10.322586	8.008942	8.138913	H27	9.692246	8.560441	6.395357
H13	10.239642	7.369984	9.023715	C28	13.225149	7.702793	10.961200
H14	10.014177	7.414608	7.276038	H29	14.106647	8.249363	11.312051
H15	9.610921	8.836935	8.261265	H30	13.422248	6.633075	11.105838
C16	14.508789	9.656404	10.351882	H31	12.378779	7.964719	11.605696
H17	15.081617	10.588949	10.302917	C32	14.745502	9.331205	6.464870
H18	15.230367	8.840978	10.489128	H33	15.743386	9.052155	6.817116
H19	13.875332	9.686956	11.244478	H34	14.663699	10.424689	6.532392
C20	14.085530	10.007139	5.371422	H35	14.680259	9.048415	5.411200
H21	14.763334	10.855162	5.510516	C36	11.396544	7.275881	2.294157
H22	13.308545	10.304271	4.657098	C37	10.199225	6.554187	2.358445
H23	14.664627	9.186272	4.929681	C38	9.859217	5.769106	1.258314
C24	11.504917	6.800088	2.551778	H39	8.929403	5.198867	1.288162
C25	10.723515	5.684267	2.229927	C40	10.667980	5.708004	0.124280
C26	11.067929	4.966606	1.086853	C41	11.836143	6.468631	0.093105
H27	10.478889	4.087110	0.823415	H42	12.469891	6.438410	-0.794016
C28	12.134706	5.341605	0.271790	C43	12.220628	7.273461	1.162500
C29	12.853140	6.490091	0.600404	C44	9.331552	6.578890	3.579078
H30	13.672780	6.812499	-0.042852	H45	8.334533	6.188227	3.353270
C31	12.552448	7.240831	1.734806	H46	9.217281	7.597329	3.972634
C32	9.557512	5.284233	3.074266	H47	9.760051	5.964982	4.384772
H33	9.096326	4.368915	2.687054	C48	10.273988	4.878942	-1.061971
H34	8.800844	6.079257	3.075101	H49	9.787883	5.494495	-1.829900
H35	9.860834	5.114202	4.115893	H50	9.568767	4.085049	-0.788088
C36	12.505586	4.517958	-0.925002	H51	11.148433	4.413456	-1.532148
H37	13.091049	5.096166	-1.647432	C52	13.460270	8.107864	1.105255
H38	11.617379	4.131206	-1.436882	H53	14.008465	7.926852	0.175659
H39	13.111267	3.650736	-0.631635	H54	14.126960	7.889549	1.950088
C40	13.364769	8.448348	2.087119	H55	13.196801	9.172253	1.153294
H41	13.967852	8.773161	1.233852	C56	12.692552	4.722608	3.625682
H42	14.048848	8.237329	2.921155	H57	11.886203	4.909736	2.912696
H43	12.728432	9.288459	2.393784	C58	10.768782	1.471937	1.917914
C44	10.545188	9.166608	5.058319	H59	10.847083	0.566486	2.541095
C45	10.199788	8.531079	3.824970	C60	9.329938	1.932156	1.886468
O46	9.342240	8.718657	2.981745	H61	8.958770	2.123430	2.897991
H47	10.114333	10.027362	5.547213	H62	8.694835	1.175978	1.412966
Ru48	13.058661	5.930463	5.601065	H63	9.255114	2.863489	1.310865
C149	10.985082	5.188909	6.423945	C64	11.322428	1.222259	0.528949
C150	15.202870	6.800379	6.109692	H65	12.378174	0.932240	0.550031
O51	11.954645	2.724213	4.753341	H66	11.234563	2.139964	-0.066204
C52	13.502041	5.042650	4.084863	H67	10.758544	0.428214	0.026583
H53	13.588171	5.560261	3.121582	C68	12.715039	2.307992	3.073410
C54	11.096292	1.584784	4.900916	C69	13.337674	1.062410	3.138161
H55	11.533234	0.899779	5.644720	H70	12.858819	0.179197	2.726286
C56	9.779260	2.099182	5.432250	C71	14.584716	0.939375	3.743289
H57	9.914895	2.606566	6.391011	H72	15.052797	-0.041945	3.785187
H58	9.079029	1.265614	5.557613	C73	15.240852	2.043936	4.274647
H59	9.343157	2.819252	4.729361	H74	16.225258	1.939661	4.722020
C60	10.937662	0.893608	3.560199	C75	14.637219	3.288568	4.197586
H61	11.894053	0.543704	3.156909	H76	15.172083	4.175488	4.542279
H62	10.501377	1.599884	2.842283	C77	13.367549	3.449206	3.611121
H63	10.266359	0.032086	3.648105	C78	11.843926	9.746728	4.841460
C64	13.280226	2.554668	4.610532	C79	11.601581	9.496008	3.459086
C65	13.941439	1.331764	4.780929	H80	11.792855	10.664022	5.408612
H66	13.390222	0.448556	5.087915	O73	11.299161	10.187692	2.503417
C67	15.305541	1.227709	4.551191	76			
H68	15.791749	0.265427	4.697669	4b - s			
C69	16.046800	2.326332	4.126188	Ru1	12.889636	5.679968	5.261517
H70	17.113825	2.238465	3.940998	C12	10.685779	4.997350	5.895130
C71	15.402460	3.538096	3.952179	C13	15.167611	6.435144	5.354760
H72	15.963554	4.421801	3.650013	O4	13.652813	3.738293	5.978608
C73	14.025210	3.682654	4.192766	N5	11.793347	8.457905	5.574468
73				N6	11.330795	7.873420	3.596242
4a - P dis				N7	12.098491	7.538887	4.658130
Ru9	13.112496	5.813403	5.030066	C8	12.470775	8.452168	6.843452
C110	11.700545	4.870695	6.682197	C9	11.831952	7.926677	7.971906
C111	15.108022	6.805393	4.207658	C10	12.574638	7.882894	9.153852

H11	12.108194	7.457743	10.044139	C15	13.644247	9.160822	6.936854
C12	13.874559	8.373622	9.228157	C16	10.344759	7.522195	8.057473
C13	14.424857	8.986596	8.101910	H17	10.316955	6.483037	8.402407
H14	15.422904	9.421406	8.160891	H18	9.860081	7.537526	7.079482
C15	13.740363	9.048567	6.895268	H19	9.759182	8.129056	8.760506
C16	10.397240	7.493902	7.991846	C20	14.532005	8.580426	10.582558
H17	10.294053	6.507412	8.457668	H21	15.109711	9.501666	10.718960
H18	9.954933	7.419490	6.995930	H22	15.245854	7.746761	10.587278
H19	9.811028	8.205216	8.589366	H23	13.876645	8.453845	11.450077
C20	14.675635	8.245761	10.488458	C24	14.236229	9.805598	5.719917
H21	15.357092	9.093257	10.620707	H25	15.133112	10.375690	5.982466
H22	15.293208	7.338202	10.460786	H26	13.526309	10.491651	5.237985
H23	14.034042	8.178290	11.373302	H27	14.514326	9.061509	4.962335
C24	14.345009	9.727249	5.706102	C28	11.634637	7.316986	2.333592
H25	15.105882	10.447169	6.023244	C29	10.625734	6.508397	1.791185
H26	13.595843	10.260183	5.107521	C30	10.867984	5.928327	0.548587
H27	14.828386	8.984439	5.059242	H31	10.101893	5.284567	0.113381
C28	11.476224	7.232577	2.332846	C32	12.056164	6.144417	-0.148785
C29	10.412900	6.454193	1.858389	C33	13.017816	6.981141	0.411942
C30	10.575473	5.830070	0.625095	H34	13.951948	7.159379	-0.123043
H31	9.762955	5.214580	0.236793	C35	12.826016	7.586726	1.650378
C32	11.743574	5.973927	-0.124402	C36	9.337483	6.282529	2.516617
C33	12.764683	6.781250	0.373663	H37	8.723201	5.540973	1.996266
H34	13.674800	6.917594	-0.211786	H38	8.773146	7.222169	2.576638
C35	12.652737	7.431047	1.602584	H39	9.511702	5.933758	3.544312
C36	9.154055	6.305529	2.652262	C40	12.285969	5.482107	-1.474372
H37	8.469249	5.602311	2.168448	H41	13.330073	5.571749	-1.793586
H38	8.651193	7.277076	2.742305	H42	11.657985	5.925280	-2.257573
H39	9.365936	5.941899	3.667461	H43	12.035206	4.414287	-1.431491
C40	11.890957	5.264494	-1.438005	C44	13.878660	8.481542	2.228518
H41	12.727638	5.663013	-2.020956	H45	14.604605	8.768934	1.461143
H42	10.981924	5.353652	-2.043867	H46	14.425909	7.979349	3.039043
H43	12.071316	4.191465	-1.292000	H47	13.442051	9.397310	2.647834
C44	13.773356	8.271521	2.132346	C48	12.764344	4.788394	3.772366
H45	14.475218	8.528279	1.332765	H49	11.835283	4.261065	3.512724
H46	14.332484	7.741194	2.918197	C50	16.377193	5.961812	5.168838
H47	13.400992	9.205014	2.573755	H51	17.075520	6.528580	4.532510
C48	13.020560	4.779176	3.673780	C52	16.128571	6.737945	6.435608
H49	12.775011	5.212237	2.698727	H53	15.763829	7.745287	6.217010
C50	13.792029	3.305523	7.363019	H54	17.067120	6.827721	6.994758
H51	14.736653	2.742930	7.409988	H55	15.396011	6.218699	7.067219
C52	13.912752	4.553619	8.204248	C56	16.894965	4.565389	5.439337
H53	14.714552	5.205051	7.838488	H57	17.102560	4.008645	4.520352
H54	14.127410	4.267734	9.240814	H58	16.155265	4.011237	6.028703
H55	12.968431	5.115726	8.199377	H59	17.827279	4.631667	6.011798
C56	12.606396	2.447594	7.747496	C60	15.101255	5.282924	3.228189
H57	12.518505	1.553897	7.120951	C61	16.185590	5.252967	2.360182
H58	11.685579	3.032534	7.638117	H62	17.123827	5.735603	2.618727
H59	12.706854	2.125958	8.790477	C63	16.066522	4.573309	1.149743
C60	13.838190	2.871706	4.947224	H64	16.921152	4.543553	0.477177
C61	14.325312	1.576890	5.054245	C65	14.883295	3.929366	0.797539
H62	14.586725	1.144163	6.015029	H66	14.810825	3.391737	-0.144819
C63	14.477883	0.829020	3.888445	C67	13.796398	3.988147	1.655891
H64	14.860461	-0.186282	3.965119	H68	12.850817	3.513559	1.396225
C65	14.150962	1.351046	2.638906	C69	13.884687	4.671852	2.875584
H66	14.276568	0.744926	1.745872	C70	10.780839	9.346358	5.174598
C67	13.666178	2.646195	2.545668	C71	10.506019	9.006521	3.811146
H68	13.403266	3.083525	1.583284	C72	10.203464	10.458799	5.955678
C69	13.503429	3.425496	3.697490	H73	9.615881	11.076408	5.269560
C70	10.897494	9.368983	5.156771	H74	9.535730	10.105467	6.752319
C71	10.536217	9.024283	3.818720	H75	10.976813	11.081962	6.422701
C72	10.445770	10.536430	5.940942	O76	9.748654	9.487767	2.981206
H73	9.838826	11.163243	5.280631				
H74	9.828122	10.248593	6.801620				
H75	11.285626	11.132814	6.319640				
O76	9.780070	9.536221	3.005500				
76							
4b - S - cis				4b - TS inter			
Ru1	12.889059	5.702445	5.341660	C1	14.394567	3.773667	7.697525
C12	10.659420	5.186710	5.854456	C2	13.493862	4.376026	8.511215
C13	13.640094	4.076511	6.857703	H3	13.665009	5.439093	8.714615
O4	15.106473	5.914200	4.444123	C4	12.363491	3.742508	9.247464
N5	11.729921	8.502747	5.609079	H5	12.456908	3.935220	10.323948
N6	11.401933	7.934912	3.595695	H6	11.405196	4.166323	8.916475
N7	12.150333	7.637394	4.685700	H7	12.316797	2.659092	9.102058
C8	12.387551	8.532032	6.889507	C8	14.486090	2.320563	7.377761
C9	11.753807	8.025931	8.027526	H9	13.588481	1.761518	7.656364
C10	12.483219	8.055283	9.220000	H10	14.663993	2.163028	6.306682
H11	12.019856	7.640735	10.115856	H11	15.342843	1.878205	7.904769
C12	13.756870	8.602965	9.300329	H12	15.199194	4.403950	7.314446
C13	14.308869	9.182653	8.154300	N13	11.412379	8.286023	5.687848
H14	15.288805	9.658778	8.212833	N14	11.294049	7.238586	3.842862
				N15	11.998260	7.294580	5.006256
				C16	11.942044	8.682067	6.969383
				C17	11.298745	8.291077	8.148013
				C18	11.927966	8.625565	9.349654



H19	11.457656	8.313112	10.283362	O12	11.370328	2.510538	2.664918
C20	13.109269	9.358258	9.389048	N13	11.917567	8.518405	5.561016
C21	13.648134	9.820226	8.188110	N14	11.570918	8.043246	3.533112
H22	14.550813	10.431622	8.205108	N15	11.816307	7.478708	4.739142
C23	13.087468	9.492725	6.961822	C16	12.143370	8.304077	6.965991
C24	9.957665	7.622444	8.198112	C17	11.034960	7.930215	7.743373
H25	10.003262	6.694240	8.779180	C18	11.250245	7.704461	9.096659
H26	9.569983	7.353435	7.213703	H19	10.408578	7.395893	9.717191
H27	9.240848	8.288999	8.695879	C20	12.508130	7.870560	9.678733
C28	13.797698	9.650007	10.687803	C21	13.556904	8.320924	8.883707
H29	14.202235	10.668210	10.709483	H22	14.533722	8.502798	9.334693
H30	14.643398	8.966217	10.835127	C23	13.403839	8.559694	7.515818
H31	13.123230	9.529831	11.541846	C24	9.668875	7.788237	7.149897
C32	13.709275	9.977851	5.690154	H25	8.903277	7.872714	7.927593
H33	14.304577	10.877473	5.874787	H26	9.570505	6.803161	6.676246
H34	12.963461	10.212732	4.920560	H27	9.470835	8.552286	6.387057
H35	14.378063	9.204525	5.291502	C28	12.719272	7.558445	11.129354
C36	11.716863	6.431189	2.744322	H29	13.575966	8.102017	11.541245
C37	10.887985	5.384606	2.315501	H30	12.912802	6.486574	11.268343
C38	11.332498	4.607064	1.249260	H31	11.835068	7.805257	11.727385
H39	10.708551	3.778626	0.909914	C32	14.564965	9.108722	6.743654
C40	12.531771	4.872591	0.590823	H33	15.416805	8.419827	6.785739
C41	13.290118	5.966959	1.002836	H34	14.884498	10.060610	7.187125
H42	14.210734	6.211769	0.470344	H35	14.346967	9.263595	5.684826
C43	12.900028	6.767537	2.074141	C36	11.280229	7.249177	2.385371
C44	9.546683	5.151668	2.931478	C37	10.103296	6.490261	2.364360
H45	9.090474	4.237388	2.537720	C38	9.862875	5.698328	1.241852
H46	8.887104	5.998583	2.700867	H39	8.953486	5.095576	1.210230
H47	9.613947	5.075713	4.023566	C40	10.742008	5.672889	0.161193
C48	12.994487	3.990055	-0.527989	C41	11.871572	6.488719	0.199566
H49	13.730270	4.493631	-1.164178	H42	12.557677	6.491224	-0.648852
H50	12.158583	3.668774	-1.159782	C43	12.161824	7.296221	1.294286
H51	13.467753	3.082119	-0.127776	C44	9.142096	6.495079	3.513314
C52	13.726890	7.947756	2.485266	H45	8.166045	6.112823	3.197820
H53	14.457672	8.195229	1.708870	H46	9.000140	7.507632	3.911921
H54	14.277524	7.761830	3.419178	H47	9.498009	5.868585	4.346271
H55	13.100152	8.832657	2.656687	C48	10.498259	4.792752	-1.028035
C56	10.414892	8.883025	5.024454	H49	10.575562	5.356796	-1.965372
C57	10.281619	8.216351	3.762430	H50	9.507824	4.325276	-0.994661
Ru58	12.832717	5.680911	6.066301	H51	11.251228	3.992447	-1.075064
C159	10.552718	4.978703	6.376977	C52	13.363026	8.186585	1.294229
C160	14.938199	6.853451	6.465343	H53	13.990306	7.988967	0.418839
O61	12.160699	2.522741	5.309614	H54	13.968704	8.039028	2.197702
C62	13.625797	4.932056	4.581986	H55	13.047830	9.237791	1.273543
H63	14.218772	5.674629	4.028164	C56	12.473469	4.752676	3.632032
C64	11.140065	1.514624	5.454886	H57	11.378162	4.719154	3.556083
H65	11.585329	0.530551	5.243151	C58	10.602631	1.389670	2.210623
C66	10.689595	1.521399	6.896474	H59	11.297145	0.583876	1.921565
H67	11.507330	1.234527	7.567078	C60	9.791785	0.951717	3.408906
H68	9.876741	0.797256	7.025353	H61	10.443946	0.664975	4.239877
H69	10.331621	2.516849	7.178132	H62	9.155417	0.098537	3.150106
C70	10.011214	1.817876	4.491283	H63	9.153787	1.776247	3.748070
H71	10.369359	1.879757	3.455892	C64	9.729155	1.788922	1.038378
H72	9.563846	2.782863	4.758350	H65	10.317456	2.155357	0.189759
H73	9.239488	1.041401	4.543755	H66	9.046565	2.590200	1.348629
C74	12.992625	2.468033	4.263127	H67	9.130145	0.936518	0.698326
C75	13.152505	1.333639	3.455042	C68	12.474632	2.912727	2.007161
H76	12.541610	0.452204	3.615275	C69	13.009900	2.277653	0.887152
C77	14.100914	1.305763	2.443153	H70	12.517351	1.416007	0.445848
H78	14.206534	0.400776	1.847640	C71	14.198798	2.745368	0.335550
C79	14.908933	2.409901	2.187499	H72	14.606187	2.239888	-0.537948
H80	15.657766	2.384617	1.399895	C73	14.875066	3.826365	0.891376
C81	14.713139	3.553569	2.937352	H74	15.807900	4.174595	0.456017
H82	15.298580	4.446960	2.724541	C75	14.353238	4.453698	2.011803
C83	13.765114	3.628165	3.980820	H76	14.854937	5.305474	2.469175
C84	9.675691	10.072450	5.492356	C77	13.133742	4.039548	2.566651
H85	9.069153	10.437877	4.658402	C78	11.729464	9.708276	4.967373
H86	9.004388	9.841305	6.329434	C79	11.489660	9.454165	3.580662
H87	10.351534	10.872331	5.820077	C82	13.342067	2.412471	5.753994
O88	9.546129	8.413606	2.806323	H83	12.704375	2.159776	4.898332
88				H84	14.023633	1.566250	5.922971
4b - P inter				H85	12.691601	2.519994	6.624546
C1	14.154662	3.638667	5.481449	H86	14.746229	3.608838	4.564558
C2	14.553530	4.588381	6.406957	C86	11.706942	11.014232	5.657736
H3	15.425662	5.190806	6.147792	H87	11.361310	11.762132	4.937499
C4	14.123343	4.664841	7.839223	H88	11.028888	11.014048	6.520671
H5	13.871718	5.698565	8.123825	H89	12.699842	11.317961	6.014333
H6	13.256330	4.038820	8.062226	O88	11.244052	10.192776	2.637031
H7	14.962940	4.363693	8.482061	76			
Ru9	12.957369	5.617767	5.198317	4b - TS dis			
C110	11.045690	4.688129	6.385309	N1	11.721920	8.527316	5.557976
C111	14.862962	6.865767	4.339487	N2	11.594990	7.969538	3.515197

N3	12.107140	7.580770	4.704340
C4	12.190376	8.474850	6.918542
C5	11.367031	7.951364	7.920129
C6	11.921776	7.840061	9.196770
H7	11.307633	7.418096	9.993413
C8	13.212336	8.273258	9.481851
C9	13.957234	8.876865	8.467576
H10	14.956349	9.253941	8.687467
C11	13.471644	8.989085	7.172115
C12	9.926264	7.598847	7.711298
H13	9.705468	6.602504	8.109653
H14	9.635432	7.585151	6.659058
H15	9.294063	8.318867	8.247906
C16	13.801159	8.102281	10.849102
H17	14.381420	8.982216	11.148882
H18	14.485563	7.244860	10.869010
H19	13.028812	7.926717	11.604800
C20	14.303679	9.611906	6.095204
H21	15.037732	10.299323	6.526744
H22	13.700412	10.166913	5.366187
H23	14.849274	8.828432	5.553587
C24	11.884914	7.259133	2.316244
C25	10.827530	6.632222	1.645636
C26	11.134555	5.906472	0.494783
H27	10.327312	5.398466	-0.033784
C28	12.437573	5.807754	0.012304
C29	13.452202	6.488772	0.685432
H30	14.471544	6.450862	0.295951
C31	13.203735	7.225338	1.841420
C32	9.424121	6.718991	2.153568
H33	8.756446	6.095236	1.552134
H34	9.070500	7.756841	2.111533
H35	9.363581	6.383850	3.198402
C36	12.756549	4.972225	-1.190762
H37	13.469543	5.476009	-1.853395
H38	11.858133	4.737805	-1.770650
H39	13.213558	4.019490	-0.891959
C40	14.321385	7.926755	2.548526
H41	15.171457	8.069597	1.873793
H42	14.671278	7.349555	3.418234
H43	14.009514	8.911504	2.918702
C44	11.013477	9.513342	4.983800
C45	10.885043	9.192790	3.595821
O46	10.351451	9.771256	2.660549
Ru47	12.593081	5.676780	5.374695
C148	10.216027	5.198402	5.480858
C149	14.872696	6.204943	5.866248
O50	13.046651	3.236570	5.914605
C51	12.715811	4.694997	3.860301
H52	12.095082	4.800141	2.960950
C53	12.450763	2.321686	6.857170
H54	13.235551	1.609937	7.161614
C55	12.051397	3.170221	8.042396
H56	12.915021	3.726336	8.425160
H57	11.655561	2.537223	8.844113
H58	11.272731	3.884653	7.742262
C59	11.284896	1.606538	6.211180
H60	11.604368	1.013721	5.346080
H61	10.546637	2.346736	5.877656
H62	10.808965	0.929504	6.929793
C63	13.756168	2.794811	4.827709
C64	14.465412	1.609234	4.726832
H65	14.360858	0.820542	5.467300
C66	15.352835	1.474099	3.660005
H67	15.934841	0.559354	3.571878
C68	15.517608	2.489894	2.721015
H69	16.223150	2.360727	1.904087
C70	14.739375	3.639393	2.793799
H71	14.775355	4.398426	2.012097
C72	13.877433	3.822801	3.877454
C73	10.536363	10.726901	5.677219
H74	10.084215	11.381501	4.925999
H75	9.778805	10.499586	6.438159
H76	11.351801	11.269915	6.172069
76			
4b - P dis			
Ru1	13.060443	5.864088	5.061664
C12	11.675620	4.947088	6.756245
C13	15.011937	6.894950	4.183428
O4	11.536228	2.504100	2.569787
N5	12.052050	8.619777	5.443929
N6	11.657680	8.079319	3.427664
N7	11.963079	7.552747	4.639925
C8	12.342348	8.448425	6.844002
C9	11.275395	8.092818	7.683943
C10	11.560957	7.890885	9.026414
H11	10.752349	7.598484	9.696873
C12	12.855339	8.026498	9.530867
C13	13.865807	8.445123	8.672765
H14	14.870986	8.605939	9.064343
C15	13.635671	8.690335	7.317370
C16	9.883725	7.910846	7.164718
H17	9.154706	8.030827	7.972039
H18	9.771148	6.898868	6.755559
H19	9.635126	8.625347	6.369999
C20	13.137916	7.722881	10.970673
H21	14.076185	8.176679	11.305438
H22	13.220684	6.639705	11.125070
H23	12.331808	8.079022	11.622075
C24	14.742144	9.257423	6.480564
H25	15.634724	8.625183	6.534767
H26	15.015017	10.250424	6.861347
H27	14.484527	9.344520	5.422569
C28	11.274381	7.257316	2.328881
C29	10.090667	6.514912	2.418446
C30	9.744502	5.719252	1.328154
H31	8.823453	5.135930	1.375717
C32	10.533247	5.667258	0.178983
C33	11.690815	6.441399	0.126114
H34	12.310376	6.416380	-0.770981
C35	12.081091	7.257630	1.185078
C36	9.240085	6.535639	3.651326
H37	8.247139	6.125200	3.442797
H38	9.113456	7.555923	4.036276
H39	9.691141	5.938885	4.457402
C40	10.119046	4.840556	-1.002024
H41	9.515137	5.432188	-1.701863
H42	9.512107	3.976570	-0.704411
H43	10.988554	4.472833	-1.559371
C44	13.308135	8.108312	1.101672
H45	13.850466	7.918382	0.170458
H46	13.985039	7.914089	1.944344
H47	13.030135	9.169693	1.133485
C48	12.643493	4.732862	3.687907
H49	11.822319	4.887173	2.983101
C50	10.903471	1.454541	1.829664
H51	11.006323	0.510991	2.389126
C52	9.442670	1.833953	1.761845
H53	9.010100	1.908642	2.764053
H54	8.878918	1.091078	1.187554
H55	9.341339	2.810088	1.271169
C56	11.533291	1.339425	0.455672
H57	12.601086	1.102206	0.509913
H58	11.424168	2.294791	-0.072742
H59	11.037667	0.558704	-0.132094
C60	12.758973	2.323570	3.103858
C61	13.431072	1.102814	3.152398
H62	12.996083	0.210800	2.711435
C63	14.669643	1.015407	3.779727
H64	15.175708	0.052691	3.810239
C65	15.269980	2.133598	4.348319
H66	16.248184	2.058385	4.184808
C67	14.619771	3.354560	4.281284
H68	15.115460	4.254024	4.652368
C69	13.355915	3.478988	3.673518
C70	11.774743	9.780036	4.832212
C71	11.504654	9.484582	3.457921
O72	11.184143	10.189172	2.513102
C73	11.686517	11.092272	5.503645
H74	11.304667	11.813728	4.775228
H75	11.010405	11.068011	6.367607
H76	12.663925	11.444254	5.857687
73			
5a - s			
Ru1	12.916105	5.742755	5.218314
C12	10.873654	4.940926	6.192682
C13	15.143733	6.576190	4.923710
O4	13.861404	3.883702	5.925369
N5	11.921517	8.569760	5.514359
N6	11.535484	8.042097	3.515180
N7	12.046482	7.559088	4.627851
C8	12.412240	8.431442	6.847220
C9	11.534380	7.993128	7.846955
C10	12.061930	7.808144	9.123204

H11	11.406026	7.448062	9.916456	H18	9.956154	6.979737	7.292731
C12	13.395086	8.099424	9.412494	H19	9.609001	8.672653	7.699396
C13	14.198296	8.650912	8.414147	C20	14.356254	8.488400	10.700770
H14	15.220532	8.948576	8.650226	H21	15.062109	9.321141	10.796867
C15	13.719958	8.854589	7.123235	H22	14.934208	7.560014	10.795266
C16	10.068724	7.851305	7.580860	H23	13.662936	8.526941	11.547304
H17	9.577724	7.285238	8.378533	C24	14.293000	9.583974	5.791214
H18	9.864225	7.339210	6.635733	H25	15.254182	10.041835	6.048181
H19	9.616854	8.851137	7.532898	H26	13.656929	10.362120	5.347320
C20	13.957552	7.835220	10.776821	H27	14.472650	8.830414	5.012380
H21	14.716201	8.576936	11.050174	C28	11.628309	7.261239	2.369880
H22	14.442383	6.850465	10.813909	C29	10.621204	6.410510	1.900110
H23	13.177270	7.842329	11.545268	C30	10.822969	5.828659	0.650668
C24	14.521940	9.601933	6.104984	H31	10.064430	5.147374	0.262885
H25	15.577217	9.644353	6.391743	C32	11.961686	6.089459	-0.112020
H26	14.138524	10.628445	6.030256	C33	12.920512	6.966091	0.389805
H27	14.467326	9.142804	5.113203	H34	13.818392	7.171817	-0.194137
C28	11.461422	7.267829	2.311203	C35	12.776149	7.571434	1.634888
C29	10.309848	6.505630	2.093031	C36	9.388369	6.128739	2.701126
C30	10.254011	5.777231	0.907614	H37	8.788480	5.349767	2.221197
H31	9.374141	5.165117	0.707094	H38	8.760572	7.023385	2.798264
C32	11.294937	5.807166	-0.022282	H39	9.635812	5.798028	3.720212
C33	12.421882	6.583816	0.247644	C40	12.145371	5.426866	-1.444095
H34	13.242651	6.605982	-0.469767	H41	13.165302	5.556934	-1.820943
C35	12.532550	7.334032	1.417565	H42	11.457363	5.838132	-2.193215
C36	9.218686	6.434544	3.115770	H43	11.941628	4.350542	-1.380718
H37	8.344616	5.912081	2.716350	C44	13.827624	8.493987	2.170381
H38	8.902503	7.433050	3.442364	H45	14.511692	8.803519	1.374340
H39	9.558813	5.896655	4.014286	H46	14.422379	7.999502	2.951071
C40	11.186950	5.031174	-1.300966	H47	13.390889	9.395694	2.618491
H41	12.171387	4.833384	-1.737532	C48	12.809498	4.732650	3.801274
H42	10.603040	5.584674	-2.047487	H49	11.906647	4.155091	3.554328
H43	10.681124	4.071628	-1.145731	C50	16.414275	5.961663	5.155125
C44	13.762863	8.126932	1.732579	H51	17.091320	6.569365	4.534246
H45	14.422773	8.183266	0.861979	C52	16.200941	6.657149	6.473090
H46	14.324767	7.666434	2.560150	H53	15.840367	7.678482	6.333446
H47	13.517708	9.149801	2.044357	H54	17.156298	6.703259	7.008338
C48	12.852798	4.745221	3.683405	H55	15.484400	6.102641	7.091322
H49	12.411330	5.080673	2.739651	C56	16.946811	4.555252	5.328765
C50	14.212526	3.541154	7.300730	H57	17.137436	4.053079	4.375488
H51	15.191079	3.041175	7.243106	H58	16.226829	3.962495	5.904381
C52	14.361947	4.840228	8.054816	H59	17.891907	4.597089	5.881746
H53	15.076676	5.507509	7.560926	C60	15.108668	5.348160	3.218773
H54	14.723212	4.619843	9.066462	C61	16.169395	5.394013	2.320969
H55	13.395397	5.356357	8.149596	H62	17.086722	5.921134	2.567329
C56	13.151857	2.633380	7.883486	C63	16.057257	4.731727	1.101118
H57	13.042737	1.702770	7.316517	H64	16.894723	4.761336	0.407434
H58	12.186532	3.152422	7.878868	C65	14.902946	4.027718	0.766612
H59	13.416485	2.375885	8.915491	H66	14.837601	3.500181	-0.181937
C60	13.969150	2.973396	4.923026	C67	13.836947	4.013073	1.651821
C61	14.555020	1.719481	5.023208	H68	12.913596	3.488994	1.407228
H62	14.972727	1.359226	5.928177	C69	13.916674	4.681995	2.880987
C63	14.600355	0.917570	3.884603	C70	10.826887	9.454756	5.154997
H64	15.060044	-0.065637	3.956333	C71	10.695718	9.030674	3.800378
C65	14.071761	1.344207	2.667660	O72	10.403191	10.389189	5.812571
H66	14.118912	0.696658	1.796332	H73	10.163578	9.475705	2.973513
C67	13.487603	2.597758	2.580519	85			
H68	13.067522	2.962087	1.643208	5a - TS inter			
C69	13.429206	3.430097	3.705207	C1	14.507269	4.141505	7.750406
C70	11.318881	9.741417	4.968805	C2	13.670502	4.910995	8.486479
C71	11.087207	9.311513	3.632010	H3	13.831027	5.996025	8.428266
O72	11.120872	10.765412	5.600350	C4	12.603205	4.472887	9.429782
H73	10.646111	9.821642	2.789217	H5	12.757011	4.929170	10.416731
73				H6	11.619685	4.807666	9.068604
5a - s - cis				H7	12.564420	3.386563	9.557884
Ru1	12.913318	5.655751	5.366748	C8	14.617138	2.654324	7.763028
C12	10.728426	5.028803	5.937472	H9	13.863925	2.170599	8.391820
C13	13.751309	4.035675	6.836350	H10	14.528776	2.240222	6.750864
O4	15.122974	5.945584	4.451316	H11	15.607140	2.362199	8.138021
N5	11.705715	8.449781	5.655660	H12	15.260405	4.669640	7.162724
N6	11.442044	7.921071	3.631748	N13	11.419315	8.303917	5.638917
N7	12.083261	7.548044	4.724842	N14	11.378323	7.442530	3.709024
C8	12.341315	8.470286	6.935294	N15	11.938952	7.300963	4.895139
C9	11.621861	8.095735	8.076803	C16	11.840537	8.479594	6.995395
C10	12.307215	8.110870	9.291152	C17	11.012978	8.050942	8.041158
H11	11.777652	7.798760	10.191302	C18	11.541277	8.102873	9.332147
C12	13.630979	8.530400	9.389793	H19	10.930653	7.741293	10.160977
C13	14.271446	9.004385	8.244030	C20	12.808916	8.619359	9.587991
H14	15.285657	9.399879	8.320319	C21	13.527223	9.186448	8.533490
C15	13.640272	8.995470	7.006211	H22	14.482945	9.671907	8.732665
C16	10.163291	7.778521	8.013531	C23	13.051858	9.151271	7.228350
H17	9.792508	7.464020	8.993638	C24	9.581003	7.676482	7.828332

H25	9.249504	6.949125	8.577201	C21	13.638153	8.344724	8.851500
H26	9.401161	7.244880	6.841906	H22	14.606509	8.571634	9.299128
H27	8.964221	8.579758	7.923618	C23	13.423969	8.639201	7.502784
C28	13.392150	8.579326	10.968359	C24	9.731794	7.787137	7.180442
H29	14.015115	9.458097	11.169235	H25	8.998757	7.676301	7.985285
H30	14.034930	7.696567	11.091021	H26	9.639556	6.916270	6.520870
H31	12.613501	8.526550	11.736745	H27	9.478610	8.689346	6.607993
C32	13.762471	9.864282	6.121365	C28	12.895540	7.416040	11.068247
H33	14.615532	10.425811	6.514394	H29	13.706896	8.010349	11.502177
H34	13.082085	10.570131	5.626596	H30	13.191194	6.360065	11.138181
H35	14.146653	9.162439	5.374052	H31	12.004379	7.542450	11.692937
C36	11.799336	6.675398	2.567229	C32	14.482102	9.362924	6.711518
C37	11.022566	5.594107	2.138704	H33	15.400178	9.480970	7.295592
C38	11.460192	4.917281	1.003045	H34	14.105434	10.359464	6.447221
H39	10.884835	4.060599	0.649828	H35	14.729136	8.840625	5.780838
C40	12.615455	5.292870	0.318134	C36	11.254442	7.279174	2.388450
C41	13.345470	6.387772	0.777871	C37	10.037949	6.591961	2.336424
H42	14.247001	6.694526	0.246362	C38	9.788995	5.823912	1.199018
C43	12.957466	7.103308	1.909081	H39	8.848690	5.274488	1.134204
C44	9.806859	5.143923	2.884458	C40	10.706390	5.743555	0.153324
H45	9.217241	4.449073	2.278501	C41	11.893033	6.470990	0.243226
H46	9.164415	5.982677	3.176817	H42	12.616901	6.414549	-0.571181
H47	10.092952	4.641415	3.820116	C43	12.191413	7.263085	1.347393
C48	13.077769	4.500608	-0.867066	C44	9.060408	6.630304	3.470090
H49	13.873875	5.014308	-1.415312	H45	8.064933	6.328887	3.129988
H50	12.255870	4.301315	-1.564211	H46	8.984225	7.632253	3.910931
H51	13.467089	3.524959	-0.545350	H47	9.365846	5.945783	4.277478
C52	13.788748	8.234685	2.430256	C48	10.446498	4.897534	-1.056818
H53	14.466811	8.605873	1.656076	H49	10.516709	5.488690	-1.977998
H54	14.398573	7.903935	3.286320	H50	9.454708	4.433834	-1.027378
H55	13.173703	9.073672	2.779765	H51	11.196641	4.097645	-1.133869
C56	10.521099	9.138853	4.914699	C52	13.459466	8.056372	1.402586
C57	10.547900	8.503554	3.637830	H53	14.138553	7.743011	0.603319
Ru58	12.835853	5.706862	5.881216	H54	13.977147	7.927517	2.361653
C159	10.595249	4.970285	6.361831	H55	13.263888	9.128302	1.274712
C160	15.032879	6.792282	5.792895	C56	12.463172	4.749196	3.601460
O61	12.208271	2.454690	5.714675	H57	11.372176	4.757894	3.473410
C62	13.379584	4.779011	4.382175	C58	10.507842	1.503172	2.041319
H63	13.886674	5.432853	3.658692	H59	11.221742	0.700070	1.795721
C64	11.277051	1.455706	6.183517	C60	9.670988	1.092272	3.231365
H65	11.757598	0.467471	6.106849	H61	10.303968	0.849376	4.090516
C66	11.004660	1.737756	7.641524	H62	9.058951	0.217616	2.985882
H67	11.909865	1.613655	8.244319	H63	9.007674	1.914934	3.523004
H68	10.251002	1.033617	8.012194	C64	9.659818	1.852974	0.835233
H69	10.631660	2.759930	7.763813	H65	10.265140	2.187873	-0.014406
C70	10.015677	1.511300	5.344830	H66	8.968169	2.663073	1.099633
H71	10.223295	1.348480	4.281035	H67	9.070051	0.986469	0.515631
H72	9.552530	2.498076	5.462514	C68	12.422467	2.980032	1.905084
H73	9.305469	0.744787	5.674920	C69	12.970387	2.346048	0.790560
C74	12.822966	2.274736	4.540531	H70	12.436376	1.546622	0.284959
C75	12.918843	1.028958	3.904343	C71	14.223290	2.736070	0.326329
H76	12.447773	0.154377	4.339552	H72	14.639424	2.234744	-0.545478
C77	13.620912	0.884169	2.717884	C73	14.950045	3.735076	0.965700
H78	13.682532	-0.101401	2.260487	H74	15.932071	4.021135	0.598308
C79	14.241462	1.975250	2.115695	C75	14.416121	4.358977	2.082749
H80	14.800386	1.859135	1.190475	H76	14.956336	5.150459	2.600778
C81	14.130132	3.211190	2.720796	C77	13.137477	4.025529	2.552764
H82	14.586196	4.084159	2.254260	C78	11.673020	9.811520	4.967504
C83	13.428298	3.409260	3.932043	C79	11.393397	9.409107	3.628035
O84	9.967682	10.118351	5.381962	C82	13.193627	2.389141	5.711218
H85	10.082788	8.779668	2.703544	H83	12.618875	2.156148	4.806542
85				H84	13.846136	1.529379	5.920760
5a - P inter				H85	12.481331	2.499652	6.531518
C1	14.044236	3.604011	5.514973	H86	14.693249	3.580154	4.637522
C2	14.400396	4.524279	6.485706	O84	11.682560	10.874687	5.565051
H3	15.292927	5.120811	6.291037	H	11.078913	9.987204	2.772471
C4	13.882394	4.586937	7.887597	73			
H5	13.652110	5.623867	8.176231	5a - TS dis			
H6	12.984078	3.985650	8.044686	N1	11.692091	8.507771	5.680170
H7	14.672112	4.246731	8.573124	N2	11.300996	7.726978	3.743740
Ru9	12.902446	5.608856	5.184197	N3	12.119409	7.573413	4.787718
C110	10.903349	4.703751	6.239465	C4	12.412798	8.781619	6.885118
C111	14.901806	6.760835	4.411063	C5	11.835217	8.437013	8.113514
O12	11.250484	2.648708	2.477254	C6	12.582170	8.689464	9.262342
N13	11.954034	8.547887	5.562279	H7	12.160504	8.415410	10.229959
N14	11.528748	8.071195	3.556154	C8	13.830563	9.304329	9.209502
N15	11.849318	7.510764	4.706331	C9	14.313663	9.732005	7.974035
C16	12.190560	8.316933	6.953770	H10	15.261045	10.269886	7.925457
C17	11.113949	7.887430	7.744058	C11	13.615006	9.495953	6.795937
C18	11.366478	7.608421	9.083182	C12	10.434705	7.919669	8.208559
H19	10.549601	7.248371	9.709216	H13	10.193927	7.642268	9.239408
C20	12.629682	7.796450	9.642731	H14	10.272727	7.045193	7.569714

H15	9.735295	8.702814	7.887539	H22	14.432454	6.943296	10.860140
C16	14.633695	9.518767	10.456847	H23	13.349450	8.161537	11.534264
H17	15.208196	10.450747	10.410243	C24	14.489632	9.620582	6.007055
H18	15.353114	8.702456	10.601380	H25	15.561763	9.621356	6.226528
H19	13.995978	9.553386	11.346727	H26	14.140962	10.661816	5.974615
C20	14.121276	10.020553	5.488551	H27	14.357432	9.187610	5.010820
H21	14.879876	10.792064	5.654772	C28	11.273258	7.275423	2.348171
H22	13.310942	10.464626	4.895276	C29	10.142813	6.469223	2.201281
H23	14.582188	9.217815	4.900313	C30	10.036681	5.747339	1.013917
C24	11.495158	6.980264	2.532438	H31	9.162817	5.112984	0.864348
C25	10.614647	5.941268	2.215708	C32	11.019623	5.810906	0.026659
C26	10.847292	5.256795	1.023486	C33	12.131885	6.629209	0.229952
H27	10.180864	4.436260	0.755230	H34	12.906857	6.679325	-0.535507
C28	11.903213	5.583836	0.174992	C35	12.283730	7.386107	1.388320
C29	12.736722	6.647498	0.522636	C36	9.135310	6.329376	3.300486
H30	13.556611	6.925629	-0.140281	H37	8.250856	5.788400	2.951004
C31	12.553652	7.366019	1.701584	H38	8.811779	7.303627	3.687430
C32	9.499937	5.525952	3.121811	H39	9.560435	5.773999	4.151331
H33	8.729536	4.984984	2.562632	C40	10.886129	5.033275	-1.248326
H34	9.029979	6.372447	3.634018	H41	10.570685	5.681877	-2.075485
H35	9.885875	4.869984	3.913969	H42	10.143632	4.231845	-1.161043
C36	12.149978	4.794896	-1.075845	H43	11.842467	4.584174	-1.540967
H37	12.703802	5.378372	-1.818649	C44	13.490476	8.241173	1.619596
H38	11.212081	4.460511	-1.532278	H45	14.087174	8.326260	0.706897
H39	12.742079	3.896383	-0.859479	H46	14.128363	7.810961	2.406451
C40	13.489696	8.471462	2.083499	H47	13.216094	9.251971	1.945838
H41	14.078240	8.796928	1.220506	C48	12.672100	4.754714	3.629622
H42	14.187309	8.138720	2.865087	H49	12.013461	4.970151	2.785978
H43	12.957820	9.343857	2.484267	C50	10.917571	1.552516	1.629768
C44	10.635378	9.300138	5.187107	H51	10.861040	0.703046	2.328789
C45	10.427303	8.737478	3.887068	C52	9.523201	2.078119	1.378056
O46	10.117230	10.243005	5.765281	H53	9.073396	2.448983	2.305098
Ru47	13.052735	5.814117	5.382337	H54	8.886091	1.288356	0.965695
C148	11.004123	5.043837	6.256064	H55	9.560483	2.903614	0.656726
C149	15.192840	6.761273	5.761894	C56	11.615833	1.151991	0.345300
O50	11.915887	2.628346	4.532771	H57	12.639339	0.804170	0.519076
C51	13.441090	4.939197	3.855256	H58	11.663133	2.017926	-0.326704
H52	13.417213	5.325736	2.830596	H59	11.062716	0.352793	-0.160738
C53	11.068811	1.540501	4.931150	C60	12.701916	2.342459	3.040856
H54	11.302384	1.279729	5.976066	C61	13.241628	1.068893	3.221229
C55	9.650600	2.056874	4.854772	H62	12.830256	0.210719	2.699228
H56	9.517075	2.924885	5.506682	C63	14.318599	0.883342	4.081932
H57	8.948394	1.270347	5.152371	H64	14.723170	-0.118817	4.207036
H58	9.418194	2.351876	3.823242	C65	14.889173	1.952030	4.764542
C59	11.271028	0.352357	4.007069	H66	15.744572	1.799354	5.416295
H60	12.301287	-0.016268	4.006371	C67	14.371543	3.222078	4.577278
H61	11.014393	0.643865	2.981332	H68	14.860616	4.079010	5.045682
H62	10.613050	-0.473094	4.301492	C69	13.267999	3.447647	3.731300
C63	13.235308	2.584380	4.779500	C70	11.196456	9.735269	5.023744
C64	13.884064	1.530651	5.435218	C71	10.911709	9.305392	3.697397
H65	13.309296	0.728452	5.886940	H	10.412437	9.805332	2.881478
C66	15.268968	1.491412	5.498241	O73	10.997748	10.749128	5.669041
H67	15.748038	0.659732	6.010698	76			
C68	16.045580	2.487855	4.911069	5b	-	s	
H69	17.130047	2.447966	4.961431	Ru1	12.918249	5.741427	5.208743
C70	15.411866	3.561246	4.313628	C12	10.869642	4.945838	6.177741
H71	15.993161	4.398895	3.931638	C13	15.148411	6.570664	4.914146
C72	14.008168	3.640506	4.230782	O4	13.858775	3.880938	5.917702
H73	9.775399	9.112056	3.111754	N5	11.925399	8.577094	5.506860
73				N6	11.543139	8.052161	3.502522
5a	-	P	dis	N7	12.052311	7.562610	4.620380
Ru1	12.920171	5.832213	5.089950	C8	12.414983	8.440252	6.839850
C12	11.138636	4.939041	6.376365	C9	11.537293	8.003282	7.839920
C13	15.100028	6.657595	4.594943	C10	12.064434	7.822649	9.117078
O4	11.633055	2.617427	2.268321	H11	11.408226	7.465061	9.911223
N5	11.858743	8.578831	5.537104	C12	13.397308	8.115688	9.406042
N6	11.391285	8.051089	3.547240	C13	14.200964	8.663526	8.406278
N7	11.966213	7.580318	4.634301	H14	15.223099	8.961710	8.641728
C8	12.411944	8.452029	6.847412	C15	13.722805	8.863029	7.114821
C9	11.576506	8.022268	7.887794	C16	10.072135	7.858422	7.572204
C10	12.148970	7.874964	9.146040	H17	9.579206	7.303804	8.376809
H11	11.526313	7.524809	9.969789	H18	9.871187	7.332114	6.633969
C12	13.488145	8.186635	9.382635	H19	9.620075	8.857266	7.508652
C13	14.252085	8.712722	8.342447	C20	13.958530	7.856857	10.771900
H14	15.278874	9.024928	8.534835	H21	14.716955	8.599575	11.043019
C15	13.726780	8.883570	7.063565	H22	14.443023	6.872160	10.813536
C16	10.106791	7.837933	7.676054	H23	13.177422	7.867398	11.539512
H17	9.653457	7.316705	8.524792	C24	14.524712	9.604179	6.092014
H18	9.888438	7.256795	6.774907	H25	15.577463	9.660652	6.385448
H19	9.627669	8.821008	7.575022	H26	14.132234	10.625817	5.999726
C20	14.083817	7.977018	10.742199	H27	14.480932	9.129442	5.106879
H21	14.943809	8.633342	10.912282	C28	11.473787	7.271344	2.304097

C29	10.322370	6.509491	2.083592	C33	12.902465	7.013400	0.364448
C30	10.267569	5.779214	0.899244	H34	13.786579	7.245457	-0.230636
H31	9.387373	5.167890	0.697610	C35	12.756781	7.612247	1.612850
C32	11.310666	5.806187	-0.028338	C36	9.430352	6.064307	2.721787
C33	12.439062	6.579830	0.243950	H37	8.849749	5.266840	2.248456
H34	13.262343	6.597876	-0.470715	H38	8.771311	6.935691	2.829465
C35	12.547741	7.331463	1.413101	H39	9.700319	5.740803	3.737420
C36	9.231534	6.437763	3.106974	C40	12.146724	5.456634	-1.463383
H37	8.346658	5.939826	2.699798	H41	13.158278	5.613385	-1.852584
H38	8.933894	7.433339	3.460113	H42	11.439109	5.852242	-2.202720
H39	9.565180	5.876028	3.993538	H43	11.971124	4.375246	-1.400765
C40	11.204045	5.029786	-1.306986	C44	13.790424	8.561829	2.136229
H41	12.188970	4.831000	-1.741932	H45	14.450812	8.897359	1.330644
H42	10.621800	5.583235	-2.054855	H46	14.412880	8.078176	2.902003
H43	10.697390	4.070609	-1.152340	H47	13.338833	9.447380	2.602149
C44	13.781356	8.117517	1.733161	C48	12.812078	4.739078	3.796981
H45	14.436488	8.187523	0.859791	H49	11.919882	4.139697	3.563157
H46	14.346368	7.642021	2.550365	C50	16.409085	6.019478	5.106810
H47	13.543600	9.135626	2.066809	H51	17.073144	6.639656	4.484139
C48	12.854648	4.743539	3.674626	C52	16.207870	6.697940	6.435646
H49	12.415733	5.079072	2.729645	H53	15.840664	7.718909	6.314132
C50	14.202984	3.539518	7.294688	H54	17.169845	6.742108	6.959067
H51	15.179638	3.035293	7.241891	H55	15.502646	6.131516	7.055798
C52	14.355080	4.839612	8.046860	C56	16.955887	4.616111	5.259276
H53	15.073002	5.503621	7.553105	H57	17.139798	4.125445	4.298747
H54	14.713123	4.620290	9.059847	H58	16.247712	4.011479	5.837335
H55	13.389922	5.359133	8.138158	H59	17.906903	4.660678	5.801730
C56	13.136385	2.637188	7.875327	C60	15.088818	5.406180	3.182345
H57	13.025149	1.706417	7.308999	C61	16.136208	5.476422	2.270705
H58	12.173418	3.160587	7.866596	H62	17.045207	6.022468	2.506652
H59	13.396278	2.379808	8.908571	C63	16.022965	4.813228	1.051407
C60	13.964791	2.969245	4.916773	H64	16.850572	4.861445	0.347037
C61	14.546580	1.713643	5.019097	C65	14.880043	4.084698	0.731516
H62	14.961460	1.353269	5.955309	H66	14.813774	3.556383	-0.216601
C63	14.591560	0.910640	3.881338	C67	13.825891	4.046155	1.630551
H64	15.048186	-0.073831	3.954595	H68	12.911297	3.501845	1.397097
C65	14.066284	1.337867	2.663306	C69	13.906928	4.715130	2.859559
H66	14.113011	0.689438	1.792622	C70	10.809507	9.434635	5.156748
C67	13.485746	2.593058	2.574138	C71	10.674560	9.030430	3.792409
H68	13.067928	2.957596	1.635858	O72	10.362675	10.377925	5.792907
C69	13.427980	3.426674	3.697842	C73	9.944083	9.740023	2.721412
C70	11.332689	9.737457	4.958414	H74	9.529541	10.653338	3.159451
C71	11.095928	9.322857	3.614482	H75	10.598147	10.018266	1.884663
O72	11.123938	10.778339	5.566126	H76	9.114211	9.152142	2.308006
C73	10.485634	10.106016	2.519090	88			
H74	10.237992	11.092256	2.923865	5b - TS inter			
H75	11.164545	10.242978	1.667149	C1	14.512635	4.122331	7.783169
H76	9.564137	9.649570	2.134302	C2	13.661668	4.885144	8.509347
76				H3	13.818298	5.970825	8.459134
5b - S - cis				C4	12.579647	4.436903	9.430517
Ru1	12.919125	5.663461	5.360467	H5	12.723954	4.872821	10.427988
C12	10.749710	5.016903	5.963629	H6	11.603502	4.784820	9.062678
C13	13.795940	4.056982	6.825485	H7	12.530756	3.348383	9.535634
O4	15.109599	5.998844	4.417752	C8	14.620264	2.635028	7.785321
N5	11.688212	8.448356	5.655955	H9	13.869831	2.151465	8.417688
N6	11.433660	7.929045	3.623048	H10	14.520439	2.228092	6.771137
N7	12.085276	7.555232	4.719495	H11	15.611996	2.336391	8.150165
C8	12.328092	8.482557	6.932509	H12	15.272519	4.655470	7.208586
C9	11.612415	8.116964	8.078686	N13	11.401490	8.256773	5.666580
C10	12.297809	8.152747	9.292630	N14	11.341582	7.373297	3.739138
H11	11.770372	7.849614	10.197205	N15	11.966628	7.281495	4.908881
C12	13.619137	8.581660	9.385035	C16	11.864080	8.480569	7.002346
C13	14.256938	9.042159	8.232285	C17	11.086207	8.054815	8.087971
H14	15.269059	9.444143	8.302602	C18	11.658225	8.152217	9.357214
C15	13.624419	9.014421	6.995376	H19	11.087012	7.794883	10.215540
C16	10.156530	7.786815	8.018578	C20	12.919347	8.709266	9.556144
H17	9.787398	7.480981	9.002070	C21	13.582796	9.269682	8.464220
H18	9.957759	6.977628	7.306917	H22	14.532413	9.783014	8.616661
H19	9.594498	8.672112	7.692973	C23	13.064163	9.187631	7.177426
C20	14.344397	8.563485	10.696570	C24	9.658152	7.637457	7.935803
H21	15.046799	9.400627	10.779313	H25	9.361146	6.951726	8.736958
H22	14.926123	7.639125	10.806145	H26	9.465169	7.142259	6.982309
H23	13.650632	8.612950	11.542255	H27	9.022904	8.531009	7.990096
C24	14.271931	9.591975	5.772278	C28	13.549314	8.713355	10.916387
H25	15.230697	10.058950	6.021903	H29	14.219730	9.569578	11.049001
H26	13.630263	10.360960	5.320394	H30	14.151645	7.806475	11.065314
H27	14.453321	8.829666	5.002513	H31	12.797012	8.738567	11.712311
C28	11.627667	7.270185	2.362957	C32	13.728099	9.879252	6.028562
C29	10.641722	6.388288	1.904230	H33	14.537463	10.522746	6.387009
C30	10.843331	5.814542	0.651134	H34	13.005723	10.503833	5.486328
H31	10.100652	5.110680	0.272724	H35	14.164083	9.156777	5.330385
C32	11.962922	6.110530	-0.126885	C36	11.784383	6.625460	2.593987

C37	11.048916	5.516518	2.162995	H30	13.462363	6.494370	11.120279
C38	11.507073	4.859761	1.023684	H31	12.280681	7.670491	11.698809
H39	10.964719	3.980937	0.672074	C32	14.496854	9.467688	6.592066
C40	12.644956	5.279602	0.335114	H33	15.450277	9.588026	7.116003
C41	13.333747	6.400671	0.795203	H34	14.091801	10.463617	6.368662
H42	14.221675	6.742770	0.262128	H35	14.688230	8.960789	5.640374
C43	12.921997	7.097418	1.930112	C36	11.219256	7.223661	2.422312
C44	9.857386	5.011674	2.912179	C37	9.997986	6.546052	2.377230
H45	9.291682	4.298372	2.304492	C38	9.761430	5.733373	1.267711
H46	9.182708	5.818087	3.222844	H39	8.817875	5.189100	1.209174
H47	10.171969	4.514586	3.841094	C40	10.697274	5.599584	0.244252
C48	13.133113	4.506691	-0.852499	C41	11.891447	6.316576	0.326468
H49	13.919569	5.043095	-1.393047	H42	12.632637	6.212779	-0.467565
H50	12.320285	4.291635	-1.555778	C43	12.176991	7.150696	1.402360
H51	13.544041	3.538822	-0.533794	C44	9.011027	6.627163	3.500530
C52	13.710580	8.261266	2.447238	H45	8.013553	6.330282	3.162212
H53	14.368614	8.660060	1.669231	H46	8.946101	7.638797	3.921176
H54	14.337648	7.954651	3.299680	H47	9.307158	5.956349	4.322827
H55	13.066476	9.075675	2.803823	C48	10.446071	4.714110	-0.939120
C56	10.436322	9.012622	4.971133	H49	10.411796	5.295022	-1.869177
C57	10.446589	8.378752	3.686983	H50	9.500568	4.168881	-0.849320
Ru58	12.858932	5.683527	5.894842	H51	11.256166	3.980524	-1.051105
C159	10.618983	4.937706	6.360431	C52	13.459130	7.920469	1.463773
C160	15.043612	6.794931	5.840829	H53	14.134604	7.601508	0.663686
O61	12.239531	2.434037	5.659522	H54	13.973101	7.775044	2.423406
C62	13.429282	4.781811	4.390936	H55	13.287120	8.998373	1.344543
H63	13.943763	5.450057	3.685243	C56	12.561494	4.726914	3.619334
C64	11.304324	1.428385	6.103344	H57	11.479092	4.762221	3.427363
H65	11.779579	0.440039	6.002343	C58	10.714738	1.352734	2.206426
C66	11.035632	1.677591	7.568239	H59	11.431178	0.540861	1.999985
H67	11.938801	1.521356	8.166793	C60	9.847130	0.975948	3.385527
H68	10.269046	0.978715	7.921500	H61	10.457443	0.755169	4.266803
H69	10.680697	2.703014	7.715250	H62	9.239723	0.095900	3.147729
C70	10.043531	1.509167	5.265996	H63	9.178716	1.807270	3.637930
H71	10.253492	1.380616	4.197736	C64	9.897407	1.672550	0.971291
H72	9.578640	2.490989	5.414562	H65	10.524700	1.982070	0.128010
H73	9.333885	0.731549	5.570316	H66	9.203687	2.492238	1.198336
C74	12.868846	2.275122	4.489560	H67	9.311598	0.800033	0.660778
C75	12.962626	1.044317	3.825321	C68	12.612338	2.848335	2.041503
H76	12.475564	0.164398	4.231097	C69	13.196008	2.170576	0.972517
C77	13.684245	0.920879	2.648011	H70	12.698919	1.321726	0.511993
H78	13.744708	-0.054086	2.168447	C71	14.438988	2.579333	0.497909
C79	14.325618	2.019811	2.083714	H72	14.884012	2.042797	-0.337669
H80	14.901833	1.920255	1.167168	C73	15.120261	3.640543	1.083741
C81	14.211622	3.243155	2.714182	H74	16.096216	3.940020	0.711019
H82	14.681532	4.122983	2.275091	C75	14.549412	4.310360	2.156039
C83	13.489303	3.419552	3.916087	H76	15.055172	5.147408	2.636111
O84	9.827698	9.973324	5.417536	C77	13.277453	3.958451	2.627658
C85	9.729126	8.814716	2.471010	C78	11.620378	9.783719	4.965190
H86	9.127737	9.688218	2.741226	C79	11.308615	9.377094	3.631173
H87	10.417798	9.101453	1.664829	C82	13.225834	2.382096	5.796871
H88	9.059449	8.042281	2.072126	H83	12.678970	2.132382	4.879808
88				H84	13.880501	1.531780	6.036482
5b - P inter				H85	12.489248	2.495421	6.595140
C1	14.070807	3.602848	5.610797	H86	14.754352	3.570445	4.760068
C2	14.385649	4.539030	6.581779	O84	11.596916	10.867059	5.533195
H3	15.282716	5.136853	6.415226	C86	10.772990	10.219353	2.541359
C4	13.811741	4.619618	7.960685	H87	10.630051	11.225802	2.947086
H5	13.545213	5.655870	8.219643	H88	11.451532	10.291401	1.681258
H6	12.922390	4.000168	8.096645	H89	9.807461	9.851347	2.170183
H7	14.582298	4.313713	8.683163	76			
Ru9	12.932608	5.591033	5.212944	5b - TS dis			
C110	10.898814	4.681826	6.198304	N1	11.692091	8.507771	5.680170
C111	14.962609	6.731349	4.500133	N2	11.300996	7.726978	3.743740
O12	11.449067	2.507956	2.628825	N3	12.119409	7.573413	4.787718
N13	11.964036	8.549490	5.559389	C4	12.412798	8.781619	6.885118
N14	11.491648	8.043347	3.568874	C5	11.835217	8.437013	8.113514
N15	11.866773	7.496868	4.716857	C6	12.582170	8.689464	9.262342
C16	12.258677	8.346468	6.942526	H7	12.160504	8.415410	10.229959
C17	11.225921	7.900678	7.780584	C8	13.830563	9.304329	9.209502
C18	11.538591	7.653772	9.113659	C9	14.313663	9.732005	7.974035
H19	10.757311	7.283791	9.778408	H10	15.261045	10.269886	7.925457
C20	12.816815	7.890269	9.619764	C11	13.615006	9.495953	6.795937
C21	13.776689	8.454570	8.780894	C12	10.434705	7.919669	8.208559
H22	14.754317	8.718166	9.186076	H13	10.193927	7.642268	9.239408
C23	13.516091	8.719383	7.437069	H14	10.272727	7.045193	7.569714
C24	9.825617	7.761722	7.272217	H15	9.735295	8.702814	7.887539
H25	9.129449	7.617639	8.104179	C16	14.633695	9.518767	10.456847
H26	9.732074	6.898832	6.602415	H17	15.208196	10.450747	10.410243
H27	9.523448	8.664224	6.724541	H18	15.353114	8.702456	10.601380
C28	13.147447	7.544165	11.040515	H19	13.995978	9.553386	11.346727
H29	13.966192	8.159836	11.428077	C20	14.121276	10.020553	5.488551

H21	14.879876	10.792064	5.654772	H25	15.675212	9.693982	7.057777
H22	13.310942	10.464626	4.895276	H26	14.348625	10.488003	6.180836
H23	14.582188	9.217815	4.900313	H27	14.995012	8.942827	5.601012
C24	11.495158	6.980264	2.532438	C28	11.261966	7.283101	2.374982
C25	10.614647	5.941268	2.215708	C29	10.043262	6.603325	2.449280
C26	10.847292	5.256795	1.023486	C30	9.682293	5.823056	1.351929
H27	10.180864	4.436260	0.755230	H31	8.735795	5.281931	1.382401
C28	11.903213	5.583836	0.174992	C32	10.498240	5.721929	0.227078
C29	12.736722	6.647498	0.522636	C33	11.699695	6.431086	0.198791
H30	13.556611	6.925629	-0.140281	H34	12.342685	6.357805	-0.678857
C31	12.553652	7.366019	1.701584	C35	12.111227	7.226722	1.264057
C32	9.499937	5.525952	3.121811	C36	9.182371	6.662664	3.672803
H33	8.729536	4.984984	2.562632	H37	8.170155	6.310683	3.452423
H34	9.029979	6.372447	3.634018	H38	9.111455	7.680127	4.078768
H35	9.885875	4.869984	3.913969	H39	9.598465	6.027626	4.469092
C36	12.149978	4.794896	-1.075845	C40	10.112368	4.855450	-0.932899
H37	12.703802	5.378372	-1.818649	H41	10.299245	5.355959	-1.889714
H38	11.212081	4.460511	-1.532278	H42	9.054789	4.572734	-0.896960
H39	12.742079	3.896383	-0.859479	H43	10.705550	3.930544	-0.936166
C40	13.489696	8.471462	2.083499	C44	13.418651	7.954257	1.230542
H41	14.078240	8.796928	1.220506	H45	13.961682	7.726497	0.308681
H42	14.187309	8.138720	2.865087	H46	14.051569	7.670173	2.082876
H43	12.957820	9.343857	2.484267	H47	13.284136	9.041969	1.280485
C44	10.635378	9.300138	5.187107	C48	12.704706	4.744014	3.549233
C45	10.427303	8.737478	3.887068	H49	11.929284	4.926968	2.802429
O46	10.117230	10.243005	5.765281	C50	10.929574	1.459278	1.694943
Ru47	13.052735	5.814117	5.382337	H51	10.956278	0.629258	2.419089
C148	11.004123	5.043837	6.256064	C52	9.505768	1.946660	1.551255
C149	15.192840	6.761273	5.761894	H53	9.110776	2.282034	2.515366
O50	11.915887	2.628346	4.532771	H54	8.865109	1.146348	1.165204
C51	13.441090	4.939197	3.855256	H55	9.467850	2.789647	0.849813
H52	13.417213	5.325736	2.830596	C56	11.525244	1.028809	0.368638
C53	11.068811	1.540501	4.931150	H57	12.574494	0.730525	0.460850
H54	11.302384	1.279729	5.976066	H58	11.474491	1.858307	-0.347308
C55	9.650600	2.056874	4.854772	H59	10.963463	0.184778	-0.046814
H56	9.517075	2.924885	5.506682	C60	12.807121	2.337657	2.924527
H57	8.948394	1.270347	5.152371	C61	13.417467	1.090610	3.059366
H58	9.418194	2.351876	3.823242	H62	12.993601	0.209840	2.587211
C59	11.271028	0.352357	4.007069	C63	14.583385	0.960390	3.807555
H60	12.301287	-0.016268	4.006371	H64	15.042532	-0.021940	3.896730
H61	11.014393	0.643865	2.981332	C65	15.173031	2.060611	4.419849
H62	10.613050	-0.473094	4.301492	H66	16.097767	1.953569	4.979525
C63	13.235308	2.584380	4.779500	C67	14.578528	3.303563	4.283518
C64	13.884064	1.530651	5.435218	H68	15.068453	4.185906	4.701420
H65	13.309296	0.728452	5.886940	C69	13.382914	3.471728	3.557687
C66	15.268968	1.491412	5.498241	C70	11.825658	9.849939	4.876178
H67	15.748038	0.659732	6.010698	C71	11.447212	9.434597	3.561218
C68	16.045580	2.487855	4.911069	O73	11.810692	10.936030	5.434873
H69	17.130047	2.447966	4.961431	C73	10.818751	10.263054	2.512005
C70	15.411866	3.561246	4.313628	H74	10.675010	11.264301	2.929618
H71	15.993161	4.398895	3.931638	H75	11.437263	10.353658	1.609604
C72	14.008168	3.640506	4.230782	H76	9.842658	9.865798	2.204242
C73	9.535605	9.249840	2.826565				
H74	9.069184	10.164832	3.204261				
H75	10.086569	9.487140	1.907076				
H76	8.740151	8.542005	2.560345				

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5b - P dis			
Ru1	13.061726	5.814643	4.991431
C12	11.486398	4.846907	6.478323
C13	15.101536	6.804139	4.270302
O4	11.666241	2.560128	2.242120
N5	12.204841	8.625832	5.468800
N6	11.633291	8.102918	3.491581
N7	12.054347	7.564110	4.632658
C8	12.485327	8.448535	6.861478
C9	11.437221	8.047998	7.703492
C10	11.724192	7.873720	9.052076
H11	10.927727	7.547982	9.721719
C12	12.993908	8.127280	9.569111
C13	13.975288	8.626874	8.716990
H14	14.949003	8.901268	9.124013
C15	13.740812	8.823984	7.357556
C16	10.043135	7.874083	7.187560
H17	9.333818	7.813238	8.018881
H18	9.950637	6.952796	6.600866
H19	9.751238	8.722771	6.554723
C20	13.284464	7.891387	11.020333
H21	14.110662	8.517600	11.373644
H22	13.567600	6.845903	11.196041
H23	12.407230	8.096980	11.643977
C24	14.750490	9.517658	6.499991