

Supporting Information

A Computational Study on Ruthenium-Catalyzed [4+1] Annulation via C–H Activation: Origin of Selectivity and Role of Internal Oxidizing Group

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Entire Free Energy Profile

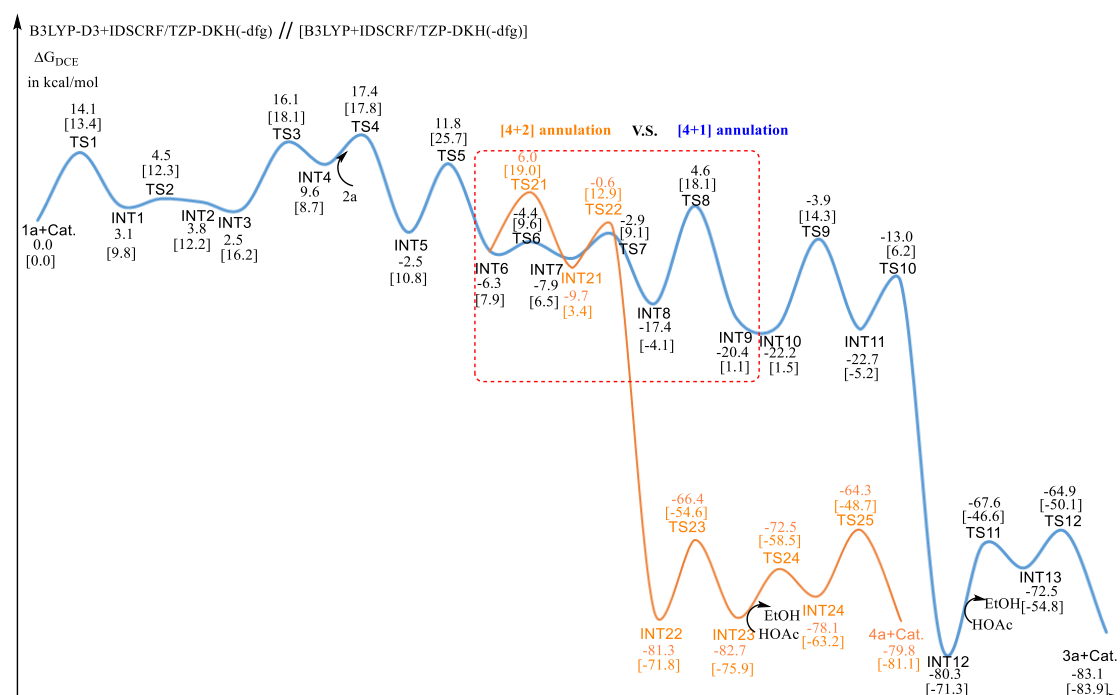


Figure S1. Whole free-energy (in kcal·mol⁻¹) of [4+2] annulation (in Yellow) and [4+1] annulation (in Blue), determined at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) and B3LYP +IDSCRF/TZP-DKH(-dfg) levels of theory in dichloroethane (DCE), respectively.

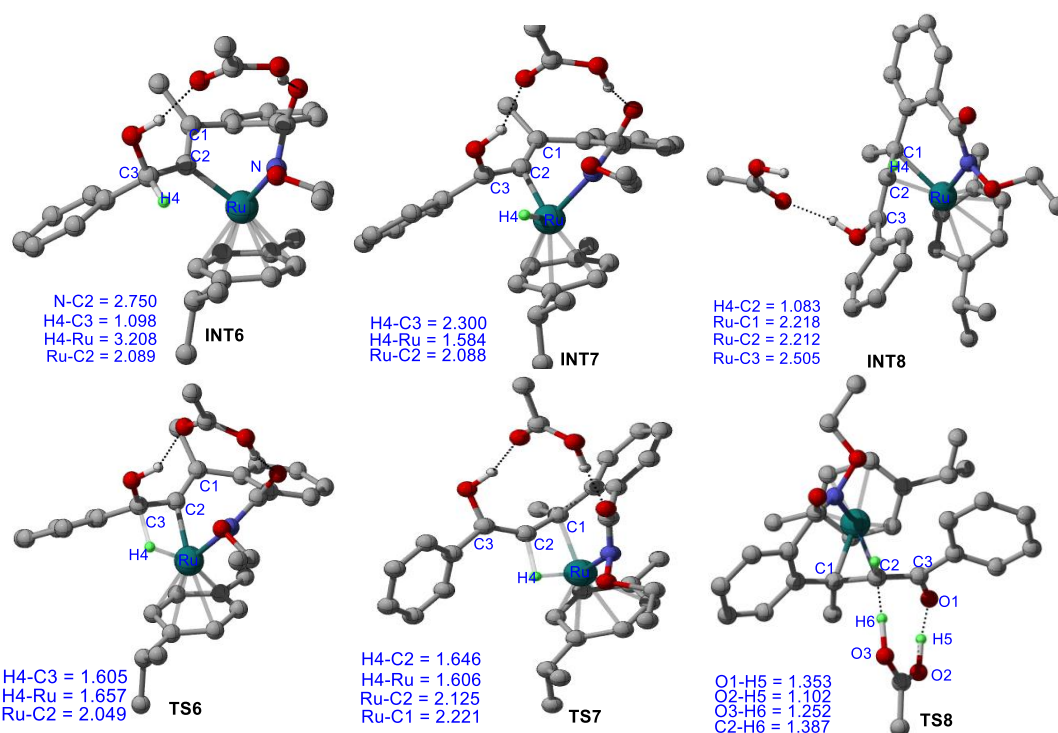


Figure S2. Geometric structures for selected transition states and intermediates of [4+1] annulation. In 3D structures, hydrogen atoms not for proton shift are omitted for clarity (distance in Å).

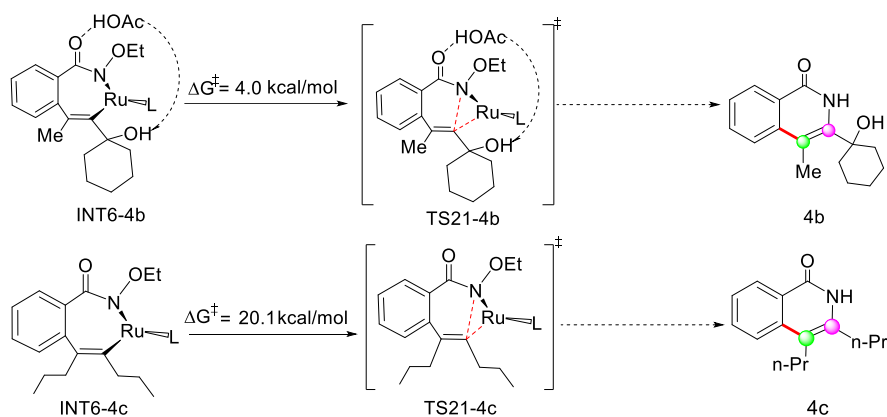


Figure S3. The relative free-energy barrier for forming **4b** and **4c** starting from **INT6**, determined at the B3LYP +IDSCRF/TZP-DKH(-dfg) levels of theory in DCE at 333K.

Computed Energies of All Stationary Points in DCE at 333K

Electronic energy calculated by B3LYP+IDSCRF/DGDZVP method (E_0 , in Hartree).

Electronic energy calculated by B3LYP+IDSCRF/TZP-DKH(-dfg) method (E_1 , in Hartree).

Total Gibbs free energy with thermal correction calculated by B3LYP+IDSCRF/TZP-DKH(-dfg) method (G_1 , in Hartree).

Electronic energy calculated by B3LYP-D3+IDSCRF/TZP-DKH(-dfg) method (E_2 , in Hartree).

Total Gibbs free energy with thermal correction calculated by B3LYP-D3+IDSCRF/TZP-DKH(-dfg) method (G_2 , in Hartree).

	E_0	E_1	G_1	E_2	G_2
1a	-554.80935	-554.92974	-554.77304	-554.95796	-554.80115
2a	-462.28852	-462.40245	-462.26317	-462.42872	-462.25918
3a	-862.16804	-862.36096	-862.11842	-862.41959	-862.17642
4a	-862.16099	-862.35753	-862.11397	-862.41511	-862.17116
HOAc	-229.1342	-229.18174	-229.13868	-229.18669	-229.14362
EtOH	-155.06988	-155.10575	-155.04278	-155.11070	-155.04771
LRu(OAc) ₂	-5289.46076	-5247.90387	-5247.63173	-5247.96146	-5247.68814
1a+cat	-5844.27563	-5802.83939	-5802.39596	-5802.93371	-5802.49031
TS1	-5844.2573	-5802.81758	-5802.37452	-5802.9136	-5802.4678
INT1	-5844.26235	-5802.82518	-5802.38032	-5802.93073	-5802.48543
TS2	-5844.25343	-5802.81731	-5802.37649	-5802.92383	-5802.48312
INT2	-5844.25787	-5802.82148	-5802.37641	-5802.93064	-5802.48425
INT3	-5844.25128	-5802.81263	-5802.37013	-5802.91849	-5802.48632
TS3	-5615.09321	-5573.61265	-5573.22838	-5573.70704	-5573.32095

INT4	-5615.11135	-5573.63007	-5573.24158	-5573.72022	-5573.33135
TS4	-6077.40022	-6036.03534	-6035.49211	-6036.15521	-6035.60832
INT5	-6077.41789	-6036.05001	-6035.50327	-6036.18572	-6035.63999
TS5	-6077.39614	-6036.02745	-6035.47945	-6036.16479	-6035.61729
INT6	-6077.42922	-6036.05685	-6035.50776	-6036.19513	-6035.6462
TS6	-6077.41867	-6036.04963	-6035.50517	-6036.18791	-6035.64312
INT7	-6077.42655	-6036.05594	-6035.51009	-6036.19442	-6035.64874
TS7	-6077.41760	-6036.05087	-6035.50588	-6036.18735	-6035.64071
INT8	-6077.44754	-6036.07731	-6035.52698	-6036.21343	-6035.66385
TS8	-6077.40753	-6036.03843	-6035.49153	-6036.17556	-6035.62881
INT9	-6077.44416	-6036.0678	-6035.51868	-6036.20741	-6035.66866
INT10	-6077.44801	-6036.07186	-6035.51813	-6036.21882	-6035.67143
TS9	-6077.42446	-6036.04803	-6035.49765	-6036.19519	-6035.6423
INT11	-6077.44798	-6036.07459	-6035.52875	-6036.21442	-6035.67222
TS10	-6077.43678	-6036.06151	-6035.51049	-6036.20831	-6035.65681
INT12	-6077.55850	-6036.18519	-6035.63411	-6036.31593	-6035.76415
TS11	-6306.67410	-6265.34256	-6264.73347	-6265.49664	-6264.88746
INT13	-6306.67959	-6265.35288	-6264.74646	-6265.50374	-6264.89534
TS12	-6151.58661	-6110.22491	-6109.69627	-6110.36571	-6109.83553
TS10b	-6077.36473	-6035.98639	-6035.43918	-6036.1253	-6035.57609
TS21	-6077.41188	-6036.03998	-6035.49013	-6036.17646	-6035.62652
INT21	-6077.44076	-6036.06668	-6035.51505	-6036.20418	-6035.65158
TS22	-6077.41928	-6036.04948	-6035.49979	-6036.18883	-6035.63706
INT22	-6077.55651	-6036.18678	-6035.63497	-6036.31886	-6035.76579
TS23	-6077.53236	-6036.16125	-6035.6075	-6036.29903	-6035.74206
INT23	-6077.56052	-6036.19153	-6035.64143	-6036.31914	-6035.7679
TS24	-6151.60361	-6110.24358	-6109.70964	-6110.3824	-6109.78252
INT24	-6151.60943	-6110.25029	-6109.71722	-6110.39143	-6109.85661
TS25	-6151.58477	-6110.22507	-6109.69401	-6110.36608	-6109.83462
TS21b	-6077.37176	-6035.99747	-6035.45069	-6036.17014	-6035.61659

**Coordinates of All Stationary Points Computed at
B3LYP+IDSCRF/TZP-DKH(-dfg) level in DCE**

1a				2a			
C	2.01459	1.17099	-0.03711	C	-2.88494	-0.36981	-0.25430
C	1.02643	0.18398	-0.04136	C	-1.88204	0.29184	-0.20543
C	1.39877	-1.15903	0.06661	C	-4.09922	-1.17331	-0.31639
C	2.74103	-1.50619	0.16568	H	-3.86515	-2.24014	-0.33437
C	3.72056	-0.51877	0.15369	H	-4.73612	-0.98441	0.55085
C	3.35463	0.82072	0.05258	H	-4.67793	-0.94046	-1.21309
C	-0.40261	0.63013	-0.13517	C	-0.67928	1.13092	-0.13946
H	1.71781	2.20959	-0.10607	O	-0.74672	2.06070	0.95892
H	3.02070	-2.54867	0.26005	C	0.61980	0.33847	-0.11067
H	4.11504	1.59258	0.04664	C	1.77035	0.90992	-0.65615
O	-0.77542	1.72783	0.24664	C	0.70944	-0.91475	0.49356
N	-1.25595	-0.31613	-0.65069	C	2.98869	0.24417	-0.59634
H	-0.88988	-0.97985	-1.32822	C	1.92895	-1.58119	0.55889
O	-2.54430	0.09564	-0.98866	C	3.07112	-1.00400	0.01413
C	-3.53587	-0.62232	-0.21985	H	1.70927	1.88319	-1.13119
H	-3.37361	-1.69668	-0.34912	H	-0.18063	-1.37601	0.90494
H	-4.47009	-0.35479	-0.71610	H	3.87306	0.69735	-1.02888
H	0.64423	-1.93534	0.10169	H	1.98504	-2.55552	1.03030
H	4.76651	-0.79170	0.22943	H	4.01970	-1.52596	0.05955
C	-3.56081	-0.23764	1.24522	H	-0.74816	1.54875	1.78700
H	-4.36263	-0.78181	1.75024	H	-0.66253	1.77402	-1.02336
H	-2.62081	-0.49123	1.73685				
H	-3.73822	0.83174	1.36385				
3a				4a			
C	-1.30270	-1.32528	0.08886	C	-0.79340	-1.02320	0.44892
C	0.04180	-1.61907	-0.64695	C	0.06702	-0.05260	0.86206
C	-1.59051	-2.32739	1.21314	C	-0.46807	-2.49474	0.43453
H	-0.81207	-2.29349	1.97243	H	-1.17202	-3.05526	1.05620
H	-2.55328	-2.10114	1.67258	H	-0.54880	-2.89777	-0.57912
H	-1.62341	-3.34337	0.81379	H	0.52763	-2.69182	0.81102
C	1.31373	-1.47416	0.17910	C	1.49863	-0.17699	1.37585
O	1.50297	-2.21868	1.12847	O	1.66418	-1.38605	2.11065
C	2.34512	-0.46108	-0.19934	C	2.53426	-0.01699	0.26944
C	3.59299	-0.52949	0.43625	C	3.42645	1.05325	0.31342
C	2.12273	0.55043	-1.14069	C	2.63110	-0.93305	-0.78125
C	4.59064	0.38275	0.13512	C	4.39566	1.21387	-0.67338
C	3.12100	1.47183	-1.43406	C	3.60021	-0.77788	-1.76323
C	4.35582	1.38815	-0.80127	C	4.48439	0.29783	-1.71366

H	3.76186	-1.31182	1.16438	H	3.36619	1.76732	1.12811
H	1.16894	0.64195	-1.64197	H	1.94840	-1.77094	-0.83297
H	5.55312	0.31411	0.62800	H	5.08048	2.05227	-0.62470
H	2.93289	2.25473	-2.15880	H	3.66484	-1.49563	-2.57265
H	5.13510	2.10368	-1.03622	H	5.23789	0.41816	-2.48301
H	0.01668	-2.66352	-0.97284	H	2.60116	-1.45394	2.36421
H	0.07228	-1.00378	-1.54218	H	1.63957	0.66668	2.06456
C	-2.73725	2.10193	0.08210	C	-3.71970	1.15953	-0.54827
C	-2.41697	0.77264	-0.15442	C	-2.46047	0.76032	-0.08235
C	-1.41592	0.11857	0.55734	C	-2.10347	-0.60768	-0.02844
C	-0.71424	0.78955	1.54888	C	-3.06679	-1.54295	-0.46349
C	-1.02839	2.12566	1.79258	C	-4.30445	-1.13600	-0.92075
C	-2.02623	2.77902	1.06656	C	-4.64051	0.22206	-0.96687
C	-3.03307	-0.18366	-1.10994	C	-1.51270	1.78108	0.35772
H	-3.52310	2.58799	-0.48367	H	-3.94591	2.21772	-0.56960
H	0.05670	0.29980	2.13146	H	-2.83958	-2.59923	-0.44157
H	-2.24975	3.81754	1.27904	H	-5.61368	0.53153	-1.32795
O	-3.94377	0.01639	-1.90559	O	-1.72038	2.99786	0.35789
N	-2.37567	-1.36015	-0.91471	N	-0.31693	1.27929	0.80716
H	-0.49012	2.66567	2.56264	H	-5.02231	-1.87958	-1.24757
H	-2.60095	-2.19138	-1.44811	H	0.33527	1.98580	1.13512
HOAc				EtOH			
H	1.88009	0.41003	0.00000	C	-1.21643	-0.24345	-0.02058
O	1.25212	-0.34451	0.00000	H	-1.26857	-0.97387	0.79148
O	-0.23213	1.33862	0.00000	H	-2.08094	0.41937	0.07051
C	0.00000	0.15129	0.00000	H	-1.29129	-0.77992	-0.96840
C	-1.03393	-0.93765	0.00000	C	0.07569	0.55486	0.04706
H	-0.90358	-1.57100	0.87924	H	0.11569	1.28259	-0.76559
H	-2.02930	-0.50273	0.00000	H	0.12815	1.11406	0.98902
H	-0.90358	-1.57100	-0.87924	O	1.24315	-0.25666	-0.11332
				H	1.29625	-0.87741	0.63067
TS1				INT1			
Ru	1.03557	-0.38061	-0.10454	Ru	-0.52756	0.18952	-0.61731
C	2.63244	0.85138	-1.04213	C	-0.34051	-1.88373	-1.33821
C	3.19982	-0.34770	-0.54163	C	-1.72223	-1.65448	-1.08927
C	2.60182	-1.57934	-0.94093	C	-2.29447	-0.52486	-1.71918
C	1.53002	-1.61223	-1.87781	C	-1.53630	0.32712	-2.56152
C	0.95483	-0.42254	-2.35195	C	-0.16642	0.05566	-2.82327
C	1.50776	0.81153	-1.88710	C	0.42623	-1.07145	-2.20620
H	2.98817	1.80560	-0.67810	H	0.15278	-2.68218	-0.79838
H	2.93602	-2.51073	-0.51043	H	-3.30409	-0.22580	-1.48247
H	1.07590	-2.56316	-2.11399	H	-1.99247	1.22607	-2.94540
H	1.00644	1.73751	-2.13303	H	1.48085	-1.26855	-2.33757
C	4.36802	-0.28049	0.41746	C	-2.49408	-2.60281	-0.19478

C	5.67076	-0.19239	-0.39976	C	-2.99667	-3.79703	-1.02506
C	4.42598	-1.42586	1.43043	C	-3.64072	-1.94147	0.57271
H	4.25531	0.65354	0.97514	H	-1.77755	-2.98042	0.54082
H	5.66146	0.65640	-1.08602	H	-2.17686	-4.30557	-1.53650
H	6.52237	-0.07494	0.27286	H	-3.49400	-4.52325	-0.37900
H	5.82677	-1.10144	-0.98587	H	-3.71532	-3.47020	-1.78119
H	3.49689	-1.49922	1.99508	H	-3.28761	-1.08465	1.14733
H	4.62554	-2.38645	0.94987	H	-4.43855	-1.60829	-0.09570
H	5.23928	-1.24353	2.13504	H	-4.08035	-2.66143	1.26537
C	-0.23225	-0.43506	-3.26764	C	0.64157	0.98492	-3.67416
H	-0.87479	0.42886	-3.09923	H	1.70350	0.90934	-3.44455
H	0.10917	-0.39950	-4.30654	H	0.49779	0.72896	-4.72804
H	-0.81920	-1.34414	-3.13817	H	0.32599	2.01696	-3.52789
C	-0.49297	-2.87894	0.60040	C	0.94465	2.74250	0.30210
O	-0.37694	-1.58387	0.72063	O	0.57316	2.00247	-0.67609
O	0.35143	-3.62146	0.10941	O	1.09480	2.36528	1.48060
C	-1.79041	-3.41720	1.17040	C	1.21805	4.18802	-0.06087
H	-1.80505	-3.25852	2.25070	H	1.65826	4.26103	-1.05442
H	-2.64060	-2.87505	0.75595	H	0.26651	4.72548	-0.08033
H	-1.88120	-4.48050	0.96055	H	1.86505	4.65460	0.67936
O	1.40587	0.12493	1.89231	O	-1.70309	1.28460	0.70755
C	0.57380	0.70942	2.67872	C	-2.67687	2.07168	0.38029
O	-0.47162	1.27995	2.32960	O	-3.10815	2.27390	-0.75637
C	0.95238	0.66753	4.14521	C	-3.29234	2.77553	1.58185
H	2.03368	0.68629	4.27151	H	-2.52509	3.33675	2.11749
H	0.49035	1.49398	4.68159	H	-4.08595	3.44752	1.26258
H	0.58292	-0.26930	4.57035	H	-3.69575	2.03712	2.27724
C	-4.29245	-0.06379	-1.20709	C	3.58177	-1.92586	-0.13040
C	-3.41281	0.59548	-0.34395	C	2.87652	-0.92393	0.54848
C	-3.51974	0.38505	1.03290	C	3.44714	0.34342	0.68253
C	-4.49658	-0.46777	1.53384	C	4.70082	0.60285	0.14059
C	-5.36305	-1.12689	0.66885	C	5.38559	-0.38962	-0.55073
C	-5.25611	-0.92653	-0.70511	C	4.82188	-1.65647	-0.68703
C	-2.44005	1.55885	-0.95504	C	1.57899	-1.31613	1.16844
H	-4.21310	0.11695	-2.27115	H	3.14610	-2.91327	-0.21198
H	-4.58019	-0.61604	2.60384	H	5.14224	1.58478	0.26099
H	-5.92915	-1.43761	-1.38332	H	5.35417	-2.43456	-1.22089
O	-2.64622	2.07471	-2.04986	O	1.34047	-2.46351	1.47665
N	-1.30439	1.79950	-0.23717	N	0.57331	-0.30462	1.34434
H	-1.12455	1.51240	0.73886	H	0.88959	0.68491	1.51248
O	-0.48415	2.85238	-0.64034	O	-0.37893	-0.67853	2.31809
C	-0.96269	4.11898	-0.12653	C	0.11648	-0.43267	3.65188
H	-0.99609	4.06303	0.96506	H	0.32232	0.63599	3.76226
H	-1.97185	4.29435	-0.50664	H	1.04497	-0.99153	3.80389

H	-2.85676	0.88832	1.72371	H	2.93145	1.12696	1.21875
H	-6.12199	-1.79239	1.06338	H	6.35924	-0.18044	-0.97803
C	-0.00152	5.18656	-0.59850	C	-0.95480	-0.89053	4.61612
H	-0.32583	6.16018	-0.22632	H	-0.62328	-0.71109	5.64057
H	1.00710	4.99781	-0.22711	H	-1.88385	-0.34236	4.45452
H	0.02873	5.23000	-1.68835	H	-1.15237	-1.95713	4.50050
TS2				INT2			
Ru	-0.44205	0.14792	-0.67514	Ru	-0.43007	-0.02544	-0.65191
C	-0.02219	-1.96209	-1.15640	C	1.49050	-0.79426	-1.45882
C	-1.42803	-1.84787	-0.93885	C	0.72923	-1.92866	-1.03449
C	-2.10652	-0.87233	-1.70077	C	-0.57841	-2.05060	-1.53727
C	-1.43129	-0.05180	-2.64313	C	-1.10385	-1.11506	-2.47838
C	-0.03963	-0.19176	-2.85030	C	-0.36006	-0.00605	-2.89990
C	0.66466	-1.17093	-2.09661	C	0.95415	0.14785	-2.34852
H	0.54163	-2.64507	-0.53382	H	2.47202	-0.62559	-1.04513
H	-3.14612	-0.65985	-1.50687	H	-1.23504	-2.82425	-1.17638
H	-1.97765	0.73397	-3.14076	H	-2.13460	-1.21797	-2.78683
H	1.73765	-1.25794	-2.19292	H	1.52462	1.03727	-2.58145
C	-2.10874	-2.76627	0.05556	C	1.35949	-2.93425	-0.09213
C	-2.36227	-4.13376	-0.60395	C	2.46425	-3.70145	-0.84337
C	-3.39556	-2.19595	0.65321	C	0.37109	-3.90965	0.54704
H	-1.39919	-2.91147	0.87529	H	1.83668	-2.36027	0.70745
H	-1.44039	-4.57325	-0.99037	H	3.21747	-3.03023	-1.25890
H	-2.78768	-4.82881	0.12266	H	2.96730	-4.39022	-0.16228
H	-3.06621	-4.04091	-1.43509	H	2.04094	-4.28624	-1.66382
H	-3.21888	-1.22093	1.10802	H	-0.43816	-3.39187	1.06158
H	-4.18371	-2.09668	-0.09738	H	-0.06831	-4.58000	-0.19573
H	-3.76871	-2.86940	1.42678	H	0.89168	-4.52971	1.27844
C	0.69048	0.70989	-3.79711	C	-0.91728	1.01132	-3.84828
H	1.70113	0.91458	-3.44561	H	-0.63389	2.02079	-3.54962
H	0.76203	0.22506	-4.77532	H	-0.52363	0.83744	-4.85386
H	0.16546	1.65545	-3.92395	H	-2.00402	0.95122	-3.89570
C	0.94230	2.76143	0.07812	C	-1.37779	2.95820	-0.04929
O	0.65464	1.99480	-0.86895	O	-0.59236	2.18495	-0.61768
O	0.95461	2.40467	1.30903	O	-2.43596	2.57331	0.60093
C	1.30751	4.18785	-0.21584	C	-1.14653	4.43843	-0.06688
H	1.45733	4.33541	-1.28211	H	-0.34679	4.69269	-0.75686
H	0.49187	4.83043	0.12445	H	-2.06613	4.95699	-0.33880
H	2.20146	4.47035	0.34016	H	-0.87322	4.76095	0.94073
O	-1.69696	1.44997	0.36916	O	-2.43818	0.12542	0.09669
C	-2.78910	2.00065	-0.05228	C	-3.45069	-0.69643	0.00236
O	-3.31694	1.84178	-1.15456	O	-3.38667	-1.83551	-0.43965
C	-3.43025	2.90899	0.98860	C	-4.75969	-0.11005	0.49987
H	-2.68068	3.54032	1.46571	H	-5.03785	0.75018	-0.11310

H	-4.20429	3.52187	0.53125	H	-5.54695	-0.85809	0.44965
H	-3.88138	2.29277	1.76985	H	-4.65341	0.24323	1.52693
C	3.37752	-1.93249	0.26959	C	3.72580	0.02065	1.35673
C	2.75113	-0.80638	0.81526	C	2.56696	0.77684	1.16537
C	3.40502	0.42419	0.75288	C	2.60632	1.86627	0.29561
C	4.64868	0.53017	0.13769	C	3.77740	2.18067	-0.38786
C	5.24610	-0.58633	-0.43421	C	4.91719	1.40113	-0.21992
C	4.60601	-1.82130	-0.36528	C	4.88789	0.31812	0.65544
C	1.45603	-1.02443	1.54999	C	1.35668	0.48496	2.01323
H	2.89499	-2.89808	0.35549	H	3.71061	-0.80281	2.06094
H	5.15219	1.48931	0.11153	H	3.79950	3.03733	-1.05180
H	5.07125	-2.70009	-0.79605	H	5.77490	-0.28782	0.79954
O	1.32441	-2.02640	2.23755	O	1.51318	0.49308	3.24546
N	0.45018	-0.06050	1.39648	N	0.17970	0.26928	1.38443
H	0.73066	1.27050	1.39312	H	-2.52504	1.54659	0.51537
O	-0.64072	-0.36119	2.26669	O	-0.88248	0.27844	2.32683
C	-0.48031	0.27182	3.54393	C	-1.17077	-1.03229	2.82057
H	-0.48548	1.35836	3.41531	H	-0.24960	-1.48701	3.19372
H	0.47704	-0.02638	3.98369	H	-1.56562	-1.64767	2.00519
H	2.96792	1.29774	1.21242	H	1.71960	2.46993	0.15996
H	6.21090	-0.49949	-0.91984	H	5.82603	1.64079	-0.75925
C	-1.63336	-0.17613	4.41731	C	-2.19013	-0.88865	3.93208
H	-1.55583	0.29438	5.39958	H	-2.45657	-1.87300	4.32261
H	-2.58933	0.10887	3.97518	H	-1.78709	-0.28993	4.75044
H	-1.62102	-1.25879	4.55204	H	-3.10097	-0.40813	3.57020
Ru(OAc) ₂ (p-cymene)				INT3			
Ru	-0.08557	-0.02259	-0.28269	Ru	-0.36014	-0.38535	-0.27434
C	1.85620	-0.22174	-1.31639	C	1.23926	-0.95690	-1.65218
C	2.08576	-0.14571	0.09533	C	0.81311	-2.19433	-1.06045
C	1.42084	-1.07559	0.92274	C	-0.55296	-2.48612	-1.10785
C	0.52395	-2.03532	0.37299	C	-1.47148	-1.60253	-1.75502
C	0.26870	-2.08984	-1.01032	C	-1.05243	-0.43324	-2.41532
C	0.96003	-1.15825	-1.85060	C	0.33809	-0.11823	-2.33572
H	2.30581	0.51579	-1.96819	H	2.26452	-0.63420	-1.52762
H	1.51033	-1.00593	1.99678	H	-0.94518	-3.35086	-0.59248
H	-0.05508	-2.65761	1.03906	H	-2.52904	-1.82708	-1.70569
H	0.72905	-1.12661	-2.90752	H	0.70411	0.80879	-2.75543
C	3.00526	0.92865	0.63765	C	1.84558	-3.08086	-0.39941
C	4.45580	0.41492	0.62197	C	2.65088	-3.80892	-1.49279
C	2.61213	1.44561	2.02343	C	1.27401	-4.07174	0.61505
H	2.93944	1.76899	-0.06034	H	2.53303	-2.41021	0.12509
H	4.75655	0.08608	-0.37465	H	3.10702	-3.10873	-2.19482
H	5.13715	1.20799	0.93569	H	3.44966	-4.39613	-1.03640
H	4.57777	-0.42707	1.30774	H	2.01019	-4.48968	-2.05871

H	1.57209	1.77441	2.04386	H	0.68489	-3.56652	1.38147
H	2.74895	0.68580	2.79628	H	0.64824	-4.82672	0.13209
H	3.24333	2.29498	2.29007	H	2.09171	-4.59969	1.10853
C	-0.72099	-3.05700	-1.58534	C	-2.01758	0.45638	-3.13820
H	-1.19637	-2.64669	-2.47666	H	-1.76817	1.50757	-2.99639
H	-0.21286	-3.98225	-1.87268	H	-1.98401	0.24458	-4.21065
H	-1.49280	-3.29499	-0.85516	H	-3.03791	0.29181	-2.79376
C	-1.40878	1.93365	-1.19295	O	1.03291	-0.08960	1.33461
O	-1.70712	0.73800	-1.50061	C	0.88919	-0.71888	2.46761
O	-0.35789	2.11983	-0.50558	O	-0.05698	-1.46054	2.72762
C	-2.27852	3.07994	-1.60396	C	1.99018	-0.47030	3.47933
H	-2.82914	2.83526	-2.51040	H	1.76553	-0.99394	4.40512
H	-2.99828	3.27676	-0.80580	H	2.94729	-0.81796	3.08649
H	-1.67940	3.97726	-1.75005	H	2.08979	0.59829	3.67400
O	-1.45226	0.33242	1.24797	C	-4.26718	1.19736	0.55839
C	-2.33985	-0.52599	1.64395	C	-2.90461	0.98181	0.74519
O	-2.50029	-1.66186	1.19735	C	-2.45557	-0.29597	1.09213
C	-3.23571	0.00996	2.75085	C	-3.35688	-1.35133	1.23998
H	-3.91205	0.75947	2.33355	C	-4.71127	-1.13213	1.03219
H	-3.82439	-0.79562	3.18457	C	-5.16277	0.14332	0.69107
H	-2.64318	0.50131	3.52311	C	-1.91791	2.09994	0.57282
				H	-4.61278	2.19165	0.30403
				H	-2.99475	-2.32499	1.54715
				H	-6.22148	0.31449	0.53446
				O	-2.20448	3.27152	0.85343
				N	-0.75356	1.64721	0.07913
				O	0.28264	2.59538	0.03082
				C	0.17059	3.46156	-1.11174
				H	-0.80195	3.95677	-1.09056
				H	0.24230	2.86526	-2.02714
				H	-1.44127	-0.45713	1.50785
				H	-5.41805	-1.94477	1.14995
				C	1.29938	4.46704	-1.03305
				H	1.25116	5.14287	-1.88931
				H	1.22386	5.06210	-0.12168
				H	2.27037	3.96927	-1.04273
				H	2.45391	0.90592	1.09092
				O	3.25833	1.48681	1.18979
				O	4.03523	0.42014	-0.62966
				C	4.17241	1.24376	0.25553
				C	5.39897	2.10033	0.42324
				H	5.87197	1.87790	1.38182
				H	6.10030	1.91192	-0.38500
				H	5.11864	3.15476	0.43870

TS3				INT4			
Ru	0.35577	0.00383	-0.28830	Ru	0.32549	0.18410	-0.34979
C	2.03043	1.05700	-1.35670	C	2.26529	1.44896	-0.35050
C	2.60271	-0.08843	-0.70358	C	2.60304	0.05543	-0.47181
C	2.04322	-1.34290	-0.98077	C	2.04209	-0.67579	-1.53207
C	0.92155	-1.46030	-1.85607	C	1.07378	-0.07352	-2.38591
C	0.35499	-0.34306	-2.49833	C	0.68682	1.27768	-2.22521
C	0.94485	0.93458	-2.22806	C	1.34479	2.04376	-1.20487
H	2.40093	2.04420	-1.11247	H	2.67989	2.02225	0.46903
H	2.41405	-2.22900	-0.48691	H	2.28010	-1.72123	-1.66211
H	0.46568	-2.43199	-1.99266	H	0.59150	-0.67376	-3.14593
H	0.49587	1.82692	-2.64356	H	1.05101	3.07275	-1.04529
C	3.77286	0.11892	0.23522	C	3.60377	-0.53128	0.50443
C	5.05761	0.33183	-0.58606	C	5.02666	-0.09951	0.10533
C	3.96138	-0.99522	1.26556	C	3.52272	-2.05058	0.66100
H	3.56560	1.04609	0.77863	H	3.38088	-0.08240	1.47777
H	4.95310	1.15612	-1.29393	H	5.11479	0.98610	0.03526
H	5.89341	0.56193	0.07741	H	5.74902	-0.44924	0.84559
H	5.31091	-0.56892	-1.15061	H	5.30196	-0.52384	-0.86344
H	3.05019	-1.17391	1.83854	H	2.51409	-2.37810	0.91769
H	4.26198	-1.93525	0.79660	H	3.82802	-2.56902	-0.25100
H	4.75070	-0.71728	1.96593	H	4.19571	-2.37505	1.45657
C	-0.81422	-0.46892	-3.42850	C	-0.32909	1.91677	-3.12455
H	-1.50447	0.36525	-3.30140	H	-0.95302	2.61502	-2.56686
H	-0.46981	-0.46636	-4.46668	H	0.17026	2.47057	-3.92513
H	-1.35670	-1.39786	-3.25540	H	-0.97400	1.16736	-3.58296
O	0.75348	1.16843	1.47723	O	0.43250	-0.13012	1.85798
C	0.35241	0.77213	2.60492	C	-0.00740	-0.94314	2.66497
O	-0.31709	-0.29122	2.76412	O	-0.74371	-1.98595	2.32994
C	0.67283	1.59772	3.82230	C	0.25006	-0.83596	4.13501
H	1.13141	0.96521	4.58318	H	0.68174	-1.76763	4.50397
H	1.33363	2.42352	3.57171	H	0.91654	-0.00322	4.33947
H	-0.25809	1.98746	4.23910	H	-0.69914	-0.68778	4.65424
C	-3.28787	-2.23839	0.13868	C	-3.42308	-1.93991	-0.58711
C	-2.31861	-1.24623	0.22015	C	-2.39275	-1.02034	-0.42601
C	-0.98889	-1.55378	0.56928	C	-1.04006	-1.38154	-0.57818
C	-0.67396	-2.89389	0.83722	C	-0.77151	-2.72046	-0.89246
C	-1.63968	-3.89021	0.74601	C	-1.80285	-3.64915	-1.05395
C	-2.94796	-3.56240	0.39581	C	-3.13018	-3.26239	-0.90439
C	-2.65366	0.17355	-0.12330	C	-2.68134	0.41004	-0.09501
H	-4.29870	-1.96268	-0.13718	H	-4.44657	-1.60553	-0.46154
H	0.33069	-3.15575	1.15171	H	0.25150	-3.06074	-1.00809
H	-3.70135	-4.33876	0.32869	H	-3.92781	-3.98502	-1.02966
O	-3.81442	0.57720	-0.28209	O	-3.82717	0.87201	0.01545

N	-1.52306	0.90034	-0.22946	N	-1.51654	1.07167	0.05071
O	-1.70410	2.21027	-0.71247	O	-1.65217	2.46945	0.18186
C	-1.89209	3.14525	0.36425	C	-1.33253	2.88720	1.51475
H	-1.02595	3.09939	1.02906	H	-0.31116	2.57404	1.75413
H	-2.78579	2.86280	0.92738	H	-2.01464	2.39816	2.21770
H	-0.49439	-0.79558	1.56789	H	-0.89170	-1.98073	1.35306
H	-1.37718	-4.92031	0.95911	H	-1.56306	-4.67865	-1.29780
C	-2.04557	4.52149	-0.24846	C	-1.47274	4.39400	1.57605
H	-2.19653	5.26257	0.53919	H	-1.23939	4.74746	2.58253
H	-1.15379	4.80011	-0.81335	H	-0.78957	4.88017	0.87682
H	-2.90566	4.55577	-0.91948	H	-2.49131	4.70121	1.33275
TS4				INT5			
Ru	2.09467	-0.13805	0.56155	Ru	1.12856	-0.96279	0.28289
C	2.23330	-1.34886	2.51878	C	0.65967	-1.72145	2.45379
C	1.86569	-2.23940	1.50876	C	0.03453	-2.65229	1.61935
C	2.66346	-2.25423	0.31185	C	0.83430	-3.18808	0.57143
C	3.84170	-1.49548	0.19029	C	2.21994	-2.93246	0.46627
C	4.17813	-0.54461	1.18112	C	2.87094	-2.09252	1.41057
C	3.31182	-0.44145	2.31210	C	2.05650	-1.44417	2.34770
H	1.62588	-1.24192	3.40583	H	0.08956	-1.20400	3.21162
H	2.35968	-2.88960	-0.51035	H	0.36935	-3.84044	-0.15689
H	4.42042	-1.55265	-0.72171	H	2.79096	-3.40750	-0.32040
H	3.52107	0.30968	3.06259	H	2.50171	-0.72285	3.02077
C	0.66896	-3.16418	1.59433	C	-1.41436	-3.07506	1.74652
C	-0.41347	-2.70064	2.57033	C	-2.27404	-2.10856	2.56196
C	1.14433	-4.59001	1.92962	C	-1.49362	-4.49945	2.32614
H	0.22968	-3.18918	0.59110	H	-1.81572	-3.10892	0.72781
H	-0.72448	-1.67462	2.36662	H	-2.19640	-1.08617	2.18876
H	-1.28742	-3.34863	2.48466	H	-3.32088	-2.41156	2.50969
H	-0.07135	-2.75623	3.60684	H	-1.98889	-2.10976	3.61713
H	1.88319	-4.95009	1.21125	H	-0.92575	-5.21262	1.72587
H	1.59535	-4.62350	2.92441	H	-1.09910	-4.52553	3.34498
H	0.29843	-5.27996	1.91734	H	-2.53173	-4.83620	2.35591
C	5.38369	0.33736	1.05883	C	4.35498	-1.89073	1.38548
H	5.22364	1.29255	1.55887	H	4.63788	-0.97916	1.91081
H	6.24417	-0.14810	1.52885	H	4.84706	-2.73408	1.87847
H	5.63434	0.52958	0.01647	H	4.73037	-1.83472	0.36422
O	-3.84846	2.09943	-0.08818	O	-2.35133	3.77648	-0.43487
C	-3.83610	2.77453	0.92913	C	-2.00906	4.61038	0.39369
O	-2.74145	3.26989	1.47954	O	-0.81037	4.68376	0.92960
C	-5.08305	3.13181	1.69291	C	-2.94491	5.67708	0.90085
H	-5.01425	2.74398	2.71099	H	-2.99423	5.64316	1.99041
H	-5.17369	4.21705	1.76499	H	-2.55859	6.66044	0.62530
H	-5.95756	2.71797	1.19843	H	-3.93671	5.54115	0.47805

C	1.39191	3.19024	-2.04501	C	3.20291	2.25265	-1.68895
C	1.41932	2.22940	-1.04317	C	2.36618	1.44678	-0.92032
C	2.40766	1.23320	-0.97925	C	2.45745	0.04558	-0.94460
C	3.38074	1.24328	-1.97825	C	3.42701	-0.51604	-1.77824
C	3.37245	2.21070	-2.98628	C	4.27431	0.28573	-2.54255
C	2.38115	3.18423	-3.02439	C	4.16478	1.67289	-2.50467
C	0.38836	2.21062	0.03030	C	1.34777	2.02879	-0.02027
H	0.60013	3.93010	-2.05386	H	3.08687	3.32897	-1.63614
H	4.16368	0.49388	-1.99466	H	3.53672	-1.59172	-1.85077
H	2.37580	3.92946	-3.81073	H	4.82047	2.29142	-3.10570
O	-0.53151	3.03713	0.10316	O	1.10086	3.26054	0.03712
N	0.61032	1.18708	0.90383	N	0.78964	1.06781	0.71532
O	-0.29208	1.14574	1.98543	O	-0.25385	1.48613	1.56455
C	0.17822	1.94482	3.08752	C	0.25620	1.91468	2.84000
H	0.26139	2.98784	2.76913	H	0.90832	2.77947	2.69396
H	1.17327	1.59409	3.37922	H	0.85164	1.10851	3.27818
H	-1.91001	3.04049	0.95622	H	-0.14685	3.98720	0.56698
H	4.14554	2.19890	-3.74737	H	5.02162	-0.18019	-3.17630
C	-0.81246	1.79501	4.22179	C	-0.92576	2.26309	3.71926
H	-0.48030	2.38446	5.07884	H	-0.57105	2.58222	4.70140
H	-1.79882	2.14972	3.92162	H	-1.50470	3.07819	3.28438
H	-0.89428	0.75263	4.53492	H	-1.58291	1.40231	3.85599
C	-0.34293	-1.72658	-3.26528	C	0.16611	-1.37073	-1.69958
C	-1.13332	-1.19064	-2.53493	C	-0.58162	-0.59033	-1.08763
C	0.61474	-2.36562	-4.15966	C	0.60816	-2.21671	-2.81436
H	0.13027	-2.70777	-5.07700	H	1.54573	-1.85067	-3.23378
H	1.41173	-1.67262	-4.43847	H	0.76125	-3.25308	-2.50588
H	1.07756	-3.23312	-3.68331	H	-0.14947	-2.20653	-3.60201
C	-2.10241	-0.55711	-1.63242	C	-1.72449	0.36685	-1.04703
O	-2.29889	0.79006	-2.06402	O	-1.34460	1.54494	-1.75232
C	-3.40880	-1.34355	-1.57622	C	-2.95593	-0.28126	-1.67012
C	-4.24130	-1.41593	-2.69428	C	-3.04674	-0.44282	-3.05368
C	-3.79202	-1.98969	-0.40441	C	-4.00959	-0.71487	-0.86938
C	-5.43267	-2.12670	-2.63875	C	-4.16789	-1.03440	-3.62137
C	-4.98485	-2.70686	-0.34667	C	-5.13387	-1.31078	-1.43579
C	-5.80723	-2.77733	-1.46429	C	-5.21425	-1.47494	-2.81346
H	-3.95292	-0.90622	-3.60594	H	-2.24336	-0.08293	-3.68494
H	-3.15815	-1.92577	0.47323	H	-3.95897	-0.57579	0.20487
H	-6.07284	-2.17510	-3.51217	H	-4.22930	-1.15043	-4.69741
H	-5.27208	-3.20332	0.57304	H	-5.94872	-1.63765	-0.80010
H	-6.73754	-3.33160	-1.42237	H	-6.08943	-1.93422	-3.25787
H	-2.77647	1.26328	-1.35542	H	-1.64264	2.32416	-1.24175
H	-1.67033	-0.55781	-0.62356	H	-1.95061	0.61585	-0.00958
TS5				INT6			

Ru	0.01598	-1.25353	0.25528	Ru	0.46499	1.08812	0.38988
C	-0.94133	-1.54979	2.29553	C	0.94741	1.29229	2.54226
C	-2.01896	-1.43153	1.40599	C	1.82545	0.32042	1.98427
C	-1.99182	-2.26950	0.25098	C	2.62264	0.73478	0.87706
C	-0.99965	-3.25687	0.09190	C	2.52381	2.03311	0.35947
C	0.00814	-3.46551	1.07760	C	1.66880	3.00273	0.97115
C	0.06121	-2.55438	2.13734	C	0.91915	2.63373	2.09720
H	-0.86281	-0.87553	3.13566	H	0.29104	1.00289	3.35043
H	-2.75856	-2.16280	-0.50496	H	3.27611	0.01888	0.39726
H	-1.02305	-3.88773	-0.78768	H	3.09069	2.30537	-0.52128
H	0.86655	-2.61501	2.85758	H	0.24932	3.34409	2.56294
C	-3.19153	-0.50338	1.64471	C	2.03058	-1.04917	2.59910
C	-2.86966	0.69817	2.53478	C	0.79504	-1.61860	3.29897
C	-4.36481	-1.31519	2.22591	C	3.22900	-0.99509	3.56493
H	-3.50238	-0.12653	0.66823	H	2.29936	-1.72457	1.78324
H	-1.99744	1.24507	2.17384	H	-0.08117	-1.60118	2.65013
H	-3.71907	1.38271	2.54894	H	0.98455	-2.65199	3.59502
H	-2.68029	0.39578	3.56791	H	0.55710	-1.06352	4.21011
H	-4.64243	-2.14551	1.57396	H	4.13377	-0.64367	3.06522
H	-4.10781	-1.72575	3.20573	H	3.02365	-0.32473	4.40356
H	-5.24015	-0.67389	2.34656	H	3.43106	-1.98897	3.96961
C	1.00484	-4.57546	0.94099	C	1.61989	4.40182	0.43400
H	1.83957	-4.44199	1.62853	H	0.69488	4.90436	0.71282
H	0.52859	-5.53407	1.16483	H	2.45637	4.97560	0.84479
H	1.39937	-4.62938	-0.07442	H	1.71117	4.41540	-0.65107
O	1.75803	3.78559	-1.04973	O	-3.09066	-2.69279	-1.11265
C	2.32965	4.34989	-0.12813	C	-4.20606	-2.62327	-0.62481
O	3.06761	3.73091	0.77126	O	-4.76068	-1.50121	-0.19722
C	2.26326	5.83948	0.09117	C	-5.10692	-3.81835	-0.44827
H	1.81607	6.04653	1.06541	H	-5.33307	-3.95454	0.61110
H	3.27087	6.25848	0.10224	H	-6.05455	-3.64826	-0.96218
H	1.67386	6.30967	-0.69148	H	-4.62707	-4.71135	-0.83971
C	4.11083	-1.21522	-1.08679	C	-1.84403	3.34088	-1.08880
C	2.83486	-0.83378	-0.68636	C	-1.47046	1.98385	-1.10764
C	1.69204	-1.55762	-1.08706	C	-0.43547	1.54458	-1.97035
C	1.89638	-2.69959	-1.87959	C	0.19337	2.51177	-2.78800
C	3.17406	-3.10014	-2.24600	C	-0.19213	3.83442	-2.76570
C	4.28775	-2.35269	-1.86448	C	-1.21879	4.25499	-1.90879
C	2.62223	0.30725	0.22966	C	-2.28938	0.99148	-0.31281
H	4.95735	-0.62134	-0.76345	H	-2.65313	3.65096	-0.43793
H	1.04504	-3.26728	-2.23719	H	0.97759	2.19141	-3.46385
H	5.28129	-2.65775	-2.16987	H	-1.52441	5.29441	-1.89661
O	3.47049	1.22563	0.38373	O	-3.47351	0.72407	-0.62016
N	1.45261	0.18257	0.85127	N	-1.55464	0.55050	0.68454

O	1.11301	1.26494	1.69070	O	-2.12121	-0.46448	1.48114
C	1.66513	1.08750	3.00639	C	-2.81426	0.10677	2.60512
H	2.75374	1.02375	2.93309	H	-3.59764	0.77659	2.23944
H	1.29319	0.14830	3.42853	H	-2.10963	0.69608	3.20080
H	3.10632	2.72002	0.61244	H	-4.14909	-0.70116	-0.31766
H	3.30187	-3.99294	-2.84771	H	0.29495	4.55084	-3.41707
C	1.24377	2.27421	3.84667	C	-3.40308	-1.02998	3.41274
H	1.64208	2.16972	4.85799	H	-3.93053	-0.62865	4.28052
H	1.62624	3.20265	3.42064	H	-4.11297	-1.60184	2.81384
H	0.15641	2.34317	3.91292	H	-2.62331	-1.70516	3.76879
C	0.36832	-0.39066	-1.87301	C	-0.12348	0.08473	-2.12366
C	-0.34606	0.31172	-1.07751	C	0.32161	-0.47081	-0.99497
C	0.55443	-0.53781	-3.34325	C	-0.33369	-0.51655	-3.49157
H	1.60827	-0.56508	-3.62187	H	-1.37309	-0.38743	-3.81202
H	0.08846	-1.45305	-3.71545	H	0.29054	-0.01531	-4.23815
H	0.07336	0.31484	-3.82583	H	-0.09982	-1.57685	-3.49707
C	-1.08412	1.61185	-1.09575	C	0.62442	-1.92868	-0.75185
O	-0.55174	2.49580	-2.09089	O	-0.22776	-2.82854	-1.48422
C	-2.57355	1.48232	-1.37387	C	2.05465	-2.35379	-1.06658
C	-3.09023	0.49341	-2.20831	C	2.89316	-1.62911	-1.91056
C	-3.44555	2.42712	-0.83145	C	2.53199	-3.54597	-0.51533
C	-4.45159	0.44624	-2.49375	C	4.17762	-2.08371	-2.20054
C	-4.80626	2.38210	-1.11107	C	3.81200	-4.00383	-0.80150
C	-5.31368	1.38910	-1.94415	C	4.64106	-3.27162	-1.64757
H	-2.42490	-0.24720	-2.63372	H	2.53961	-0.69954	-2.33784
H	-3.05313	3.20369	-0.18402	H	1.88751	-4.12235	0.13953
H	-4.83893	-0.32916	-3.14462	H	4.81621	-1.50661	-2.85961
H	-5.47096	3.12096	-0.67865	H	4.16417	-4.93113	-0.36434
H	-6.37446	1.35050	-2.16243	H	5.64093	-3.62486	-1.87123
H	0.28693	2.85842	-1.75255	H	-1.15448	-2.62519	-1.27023
H	-0.96819	2.07657	-0.11076	H	0.46363	-2.11813	0.31525
TS6				INT7			
Ru	-0.75918	0.29094	-0.53411	Ru	0.73975	0.00315	0.52139
C	-1.49388	0.39643	-2.74042	C	1.41563	-0.15868	2.72690
C	-2.54444	-0.15193	-1.99778	C	2.42905	-0.76328	1.96439
C	-2.96682	0.57023	-0.83906	C	2.97685	-0.00258	0.89681
C	-2.41151	1.81828	-0.50447	C	2.57925	1.33180	0.68541
C	-1.40664	2.42092	-1.31720	C	1.69334	2.00217	1.57970
C	-0.92103	1.65747	-2.38629	C	1.07127	1.21541	2.54722
H	-1.08863	-0.13411	-3.58937	H	0.91016	-0.71818	3.50028
H	-3.73136	0.14451	-0.20220	H	3.70794	-0.45210	0.23819
H	-2.76971	2.33801	0.37436	H	3.01725	1.88170	-0.13625
H	-0.09044	2.03070	-2.97187	H	0.31246	1.64840	3.18704
C	-3.25486	-1.43838	-2.36980	C	2.95756	-2.15819	2.23323

C	-2.36758	-2.47022	-3.06762	C	1.92214	-3.13491	2.79151
C	-4.49457	-1.10805	-3.22064	C	4.18109	-2.05820	3.16316
H	-3.60460	-1.87959	-1.43148	H	3.30170	-2.54869	1.27113
H	-1.48223	-2.69830	-2.47288	H	1.04812	-3.19858	2.14274
H	-2.92637	-3.39586	-3.21715	H	2.36221	-4.13057	2.87046
H	-2.04249	-2.12734	-4.05278	H	1.59015	-2.84903	3.79239
H	-5.15519	-0.40342	-2.71187	H	4.94673	-1.39810	2.75137
H	-4.20259	-0.66710	-4.17706	H	3.89373	-1.67270	4.14455
H	-5.06401	-2.01659	-3.42665	H	4.62597	-3.04506	3.30470
C	-0.90342	3.80254	-1.02732	C	1.43921	3.47336	1.45130
H	0.10522	3.94771	-1.41097	H	0.50347	3.76011	1.92828
H	-1.55732	4.54089	-1.50176	H	2.25054	4.03159	1.92869
H	-0.89652	4.00232	0.04366	H	1.40093	3.77702	0.40523
O	2.85524	-2.22032	1.84826	O	-2.91240	-1.67180	-2.25750
C	3.73019	-2.82962	1.24829	C	-3.88658	-2.26579	-1.81779
O	4.23756	-2.45244	0.09360	O	-4.44016	-2.02216	-0.64759
C	4.34524	-4.10186	1.77264	C	-4.58566	-3.36355	-2.57846
H	5.42506	-3.97834	1.87197	H	-4.53345	-4.29324	-2.00834
H	3.91118	-4.36197	2.73437	H	-5.64184	-3.11756	-2.70043
H	4.17621	-4.91111	1.05961	H	-4.12123	-3.50276	-3.55105
C	2.97356	2.71929	-1.07360	C	-2.71178	2.62381	1.69694
C	2.29119	1.82226	-0.24871	C	-2.12866	1.88757	0.66326
C	1.75253	2.27535	0.96999	C	-1.54542	2.55942	-0.42491
C	1.95505	3.61002	1.33825	C	-1.61266	3.95754	-0.46097
C	2.62145	4.49659	0.50419	C	-2.18353	4.68101	0.57611
C	3.12224	4.05236	-0.71562	C	-2.72331	4.01153	1.67007
C	2.36729	0.36020	-0.63078	C	-2.35683	0.39510	0.68684
H	3.41123	2.35634	-1.99602	H	-3.18222	2.09567	2.51790
H	1.56512	3.96225	2.28610	H	-1.19016	4.48728	-1.30635
H	3.64614	4.73485	-1.37439	H	-3.17256	4.56588	2.48558
O	3.52800	-0.12886	-0.71587	O	-3.56060	0.01958	0.64192
N	1.24213	-0.28637	-0.90288	N	-1.30937	-0.40697	0.82060
O	1.47139	-1.65153	-1.24869	O	-1.69595	-1.77983	0.87453
C	1.73541	-1.78530	-2.65170	C	-2.00579	-2.16322	2.21981
H	2.63290	-1.21577	-2.90836	H	-2.83955	-1.55929	2.58918
H	0.89191	-1.37754	-3.21743	H	-1.13508	-1.97854	2.85704
H	3.82708	-1.57350	-0.23528	H	-3.96326	-1.27098	-0.14322
H	2.74907	5.53023	0.80382	H	-2.20617	5.76357	0.53195
C	1.92638	-3.25892	-2.94530	C	-2.36858	-3.63396	2.20691
H	2.12326	-3.40112	-4.01000	H	-2.60456	-3.96536	3.22034
H	2.77122	-3.65881	-2.38278	H	-3.23989	-3.81149	1.57498
H	1.03388	-3.83004	-2.68301	H	-1.54046	-4.23896	1.83296
C	1.01409	1.33670	1.85123	C	-0.89308	1.80077	-1.52046
C	0.04739	0.59051	1.32397	C	-0.03379	0.82718	-1.23865

C	1.42500	1.25135	3.30216	C	-1.24550	2.16552	-2.94494
H	2.48879	1.01333	3.39032	H	-2.32572	2.10310	-3.10342
H	1.26734	2.20454	3.81523	H	-0.94663	3.19066	-3.18126
H	0.85488	0.48849	3.83120	H	-0.75205	1.50091	-3.65305
C	-0.59975	-0.62918	1.66614	C	0.58184	-0.26091	-1.84976
O	0.14746	-1.73160	1.99284	O	-0.15939	-1.31021	-2.31034
C	-1.94210	-0.68084	2.33268	C	1.94099	-0.24265	-2.44942
C	-2.51198	0.47328	2.86931	C	2.58048	0.96922	-2.72523
C	-2.61065	-1.89876	2.47389	C	2.56930	-1.43542	-2.82241
C	-3.73369	0.41365	3.53024	C	3.82553	0.98906	-3.34153
C	-3.83282	-1.95674	3.13120	C	3.81522	-1.41382	-3.43527
C	-4.39943	-0.80064	3.66105	C	4.45052	-0.20265	-3.69574
H	-1.99063	1.41748	2.77250	H	2.09042	1.89893	-2.46335
H	-2.16824	-2.80024	2.06932	H	2.07587	-2.37856	-2.62878
H	-4.16243	1.31632	3.94939	H	4.30394	1.93787	-3.55483
H	-4.34355	-2.90718	3.23263	H	4.29138	-2.34654	-3.71459
H	-5.35157	-0.84736	4.17611	H	5.42084	-0.18753	-4.17765
H	1.08885	-1.63075	1.74058	H	-1.09982	-1.23471	-2.04888
H	-0.96157	-1.14545	0.20206	H	0.73541	-1.48603	0.06182
TS7				INT8			
Ru	-1.15725	-0.80595	-0.24859	C	1.74497	-0.16412	-0.32943
C	-3.00753	-1.32681	1.03595	C	0.89372	0.56579	0.59146
C	-3.46829	-0.48603	0.01287	C	2.37064	0.54821	-1.51769
C	-3.15514	-0.85925	-1.32831	H	3.23948	1.14311	-1.21890
C	-2.48722	-2.06382	-1.60487	H	2.71065	-0.16707	-2.26742
C	-2.11627	-2.97185	-0.56905	H	1.67500	1.22054	-2.00621
C	-2.33297	-2.54981	0.74517	C	-0.01093	1.59976	0.37032
H	-3.15110	-1.05191	2.06992	O	0.04837	2.47869	-0.66935
H	-3.45335	-0.21744	-2.14754	C	-0.97746	2.02095	1.41656
H	-2.27676	-2.31996	-2.63423	C	-1.47302	3.33215	1.40292
H	-1.98596	-3.16170	1.56793	C	-1.39421	1.16552	2.44770
C	-4.29539	0.75846	0.26478	C	-2.33609	3.77985	2.39683
C	-4.03426	1.42783	1.61411	C	-2.24731	1.61967	3.44149
C	-5.78678	0.41186	0.09732	C	-2.72312	2.92918	3.42447
H	-4.03153	1.47214	-0.52100	H	-1.16803	4.00264	0.61237
H	-2.97314	1.63149	1.75914	H	-1.08211	0.13099	2.46137
H	-4.57721	2.37312	1.66526	H	-2.70192	4.79969	2.36693
H	-4.38405	0.81010	2.44507	H	-2.55503	0.94075	4.22816
H	-5.99399	-0.02195	-0.88276	H	-3.39480	3.27691	4.20048
H	-6.10715	-0.30336	0.85891	H	0.96781	2.72257	-0.89319
H	-6.39399	1.31291	0.20315	H	0.87521	0.19785	1.60450
C	-1.48986	-4.29804	-0.88208	Ru	-0.33555	-0.77084	-0.70548
H	-0.92986	-4.67975	-0.02885	C	-2.38178	-1.61162	-1.40552
H	-2.26570	-5.02776	-1.13183	C	-2.40184	-0.24619	-1.69555

H	-0.81549	-4.23198	-1.73626	C	-1.30075	0.27479	-2.45490
O	4.25128	0.98670	-0.61987	C	-0.28571	-0.55613	-2.94754
C	4.98112	1.13725	0.34840	C	-0.25482	-1.94815	-2.64123
O	4.60662	0.95880	1.60027	C	-1.30105	-2.43781	-1.83589
C	6.42566	1.54917	0.22601	H	-3.14217	-2.04564	-0.77460
H	6.69053	1.68815	-0.81872	H	-1.24904	1.33849	-2.64676
H	6.59189	2.47612	0.77794	H	0.51518	-0.12391	-3.53145
H	7.06584	0.78682	0.67371	H	-1.28021	-3.47364	-1.52624
C	3.18352	-2.17303	1.06371	C	-3.52153	0.68731	-1.28416
C	2.13173	-1.45975	0.48754	C	-4.34499	0.18775	-0.09642
C	1.71369	-1.74703	-0.82656	C	-4.42469	0.98057	-2.49632
C	2.38508	-2.78126	-1.50143	H	-3.04745	1.62961	-0.99102
C	3.41552	-3.49899	-0.91110	H	-3.70791	-0.06529	0.75151
C	3.82540	-3.19473	0.38014	H	-5.04446	0.96324	0.22061
C	1.48285	-0.44456	1.36870	H	-4.93539	-0.69361	-0.36022
H	3.48509	-1.92092	2.07206	H	-3.85598	1.38337	-3.33655
H	2.10829	-3.03074	-2.51435	H	-4.92731	0.07058	-2.83390
H	4.62991	-3.74638	0.85134	H	-5.19119	1.71061	-2.22761
O	2.19511	0.26283	2.13057	C	0.81164	-2.85307	-3.18379
N	0.14911	-0.45849	1.37693	H	0.53226	-3.21533	-4.17789
O	-0.39358	0.46612	2.31607	H	1.76572	-2.33391	-3.27705
C	-0.46796	-0.13063	3.61793	H	0.95360	-3.71973	-2.53827
H	0.53010	-0.44714	3.93074	C	3.09667	-2.97308	1.90339
H	-1.11342	-1.01554	3.57345	C	2.18580	-2.07992	1.33009
H	3.63311	0.65119	1.69753	C	2.61094	-1.21583	0.29150
H	3.90356	-4.28932	-1.46959	C	3.94494	-1.34578	-0.13665
C	-1.02299	0.90734	4.57126	C	4.82559	-2.26061	0.42130
H	-1.09714	0.48358	5.57494	C	4.40449	-3.08010	1.45944
H	-0.36896	1.77965	4.61518	C	0.79233	-2.18218	1.90150
H	-2.01726	1.23625	4.26477	H	2.73909	-3.59763	2.71061
C	0.64956	-0.98153	-1.52766	H	4.31798	-0.70762	-0.92268
C	0.30624	0.36038	-1.24623	H	5.08022	-3.79511	1.91364
C	0.37819	-1.38485	-2.97326	O	0.64637	-2.56069	3.08118
H	1.26960	-1.20549	-3.58276	N	-0.21393	-1.94198	1.04459
H	0.11457	-2.43793	-3.08335	O	-1.49392	-2.13497	1.65348
H	-0.42705	-0.78184	-3.38771	C	-1.84149	-3.52393	1.71782
C	0.75403	1.59062	-1.49804	H	-1.07876	-4.06289	2.28312
O	2.00417	1.78121	-2.05682	H	-1.88069	-3.93615	0.70349
C	0.03056	2.86217	-1.27268	H	5.84295	-2.31779	0.05103
C	-1.33462	2.99078	-1.54893	C	-3.19048	-3.62645	2.40049
C	0.72540	3.98527	-0.80805	H	-3.49950	-4.67240	2.45699
C	-1.99352	4.19588	-1.33511	H	-3.13991	-3.22916	3.41569
C	0.06632	5.18788	-0.59115	H	-3.95572	-3.07328	1.85234
C	-1.29722	5.29783	-0.85006	H	2.64643	4.06507	0.93517

H	-1.87510	2.14683	-1.95750	O	3.24470	4.71582	0.50728
H	1.78717	3.90453	-0.61517	O	2.36024	3.85182	-1.36779
H	-3.04991	4.27855	-1.56326	C	3.11632	4.63082	-0.82139
H	0.61861	6.04349	-0.22006	C	4.00738	5.59668	-1.54303
H	-1.80977	6.23833	-0.68591	H	3.77676	6.61579	-1.22766
H	2.67921	1.26523	-1.57652	H	5.04865	5.40259	-1.27951
H	-0.99323	0.76782	-0.28252	H	3.86996	5.49813	-2.61588
TS8				INT9			
C	1.69111	-0.05590	-0.59016	C	1.02883	1.20916	0.08097
C	0.94759	0.89432	0.34623	C	1.47708	0.23028	-1.07100
C	2.24958	0.56444	-1.86392	C	2.14336	1.28212	1.12240
H	3.15741	1.14759	-1.67782	H	3.09676	1.58333	0.67031
H	2.51648	-0.20958	-2.58388	H	1.91370	2.00119	1.90983
H	1.52604	1.22631	-2.32712	H	2.31034	0.31442	1.58651
C	-0.04504	1.90145	0.01900	C	1.61936	-1.24594	-0.76072
O	0.03738	2.62915	-1.02305	O	2.40980	-1.63293	0.09937
C	-1.04044	2.30878	1.05885	C	0.88311	-2.26702	-1.56376
C	-1.61604	3.58136	0.95135	C	1.30350	-3.60224	-1.46769
C	-1.39798	1.49865	2.14420	C	-0.18106	-1.95609	-2.41881
C	-2.51259	4.03826	1.90737	C	0.68453	-4.59437	-2.20974
C	-2.29305	1.95931	3.09964	C	-0.80663	-2.95451	-3.15511
C	-2.85109	3.22956	2.98759	C	-0.37421	-4.27180	-3.05689
H	-1.34348	4.20730	0.11269	H	2.12903	-3.84110	-0.81064
H	-1.00700	0.49538	2.23716	H	-0.54854	-0.94445	-2.50502
H	-2.94395	5.02777	1.81189	H	1.02741	-5.61944	-2.13448
H	-2.56176	1.31911	3.93141	H	-1.63423	-2.69932	-3.80574
H	-3.54947	3.58474	3.73637	H	-0.85877	-5.04682	-3.63927
H	1.25669	3.28741	-1.13955	H	4.00452	-1.16269	0.61482
H	0.87273	0.54027	1.36321	H	0.84192	0.36515	-1.93758
Ru	-0.30764	-0.73769	-0.80370	Ru	-0.82788	0.40976	0.92376
C	-2.39141	-1.68926	-1.31218	C	-2.59814	-0.60011	2.02490
C	-2.49418	-0.34695	-1.66316	C	-1.49211	-1.47764	1.97465
C	-1.45750	0.18890	-2.50256	C	-0.24808	-1.03495	2.53106
C	-0.45206	-0.62041	-3.04924	C	-0.11462	0.25215	3.06608
C	-0.32369	-1.98394	-2.66465	C	-1.16763	1.19263	2.95864
C	-1.28101	-2.47339	-1.74678	C	-2.41560	0.72904	2.43633
H	-3.09309	-2.12845	-0.61991	H	-3.54509	-0.89329	1.59850
H	-1.46771	1.24467	-2.74164	H	0.60596	-1.69969	2.51606
H	0.27702	-0.18315	-3.71684	H	0.84316	0.57184	3.44989
H	-1.18196	-3.48741	-1.38452	H	-3.23088	1.43443	2.33981
C	-3.63580	0.55317	-1.23792	C	-1.59511	-2.89986	1.46136
C	-4.40673	0.05091	-0.01662	C	-2.72522	-3.12824	0.45572
C	-4.58480	0.78451	-2.42862	C	-1.72105	-3.86210	2.65815
H	-3.19109	1.51994	-0.98061	H	-0.64740	-3.11806	0.96042

H	-3.74008	-0.15447	0.82132	H	-2.68795	-2.40922	-0.36274
H	-5.12938	0.80509	0.29964	H	-2.64213	-4.13121	0.03430
H	-4.96647	-0.86025	-0.24353	H	-3.70631	-3.05705	0.93218
H	-4.05757	1.19012	-3.29404	H	-0.88970	-3.75284	3.35682
H	-5.06120	-0.15142	-2.73134	H	-2.64990	-3.68200	3.20496
H	-5.37072	1.49050	-2.15214	H	-1.73177	-4.89513	2.30519
C	0.73629	-2.87680	-3.23801	C	-1.02290	2.60071	3.45367
H	0.38571	-3.32374	-4.17339	H	-1.32871	2.65969	4.50300
H	1.65029	-2.32495	-3.45790	H	0.00945	2.94314	3.38660
H	0.97877	-3.68654	-2.54993	H	-1.65238	3.28423	2.88364
C	3.31215	-2.44556	1.93135	C	-0.35695	3.91919	-2.24392
C	2.32714	-1.69409	1.28285	C	-0.22684	2.71180	-1.55596
C	2.65243	-0.96254	0.11651	C	0.76801	2.54750	-0.56757
C	3.96860	-1.09001	-0.36511	C	1.55989	3.66969	-0.28097
C	4.92382	-1.87146	0.26732	C	1.39614	4.88259	-0.94074
C	4.60173	-2.54685	1.43695	C	0.44518	5.01039	-1.94314
C	0.96071	-1.80675	1.90193	C	-1.26893	1.68791	-1.88390
H	3.02645	-2.96713	2.83466	H	-1.11936	3.99175	-3.00844
H	4.26725	-0.56035	-1.25612	H	2.33295	3.60433	0.46965
H	5.33965	-3.15124	1.95109	H	0.32098	5.94526	-2.47622
O	0.85283	-2.05257	3.11925	O	-1.77075	1.62734	-3.00760
N	-0.06484	-1.72635	1.03682	N	-1.70005	0.93231	-0.81744
O	-1.32398	-1.95089	1.67636	O	-2.91154	0.24874	-1.11347
C	-1.56665	-3.34936	1.87744	C	-4.04638	1.12823	-1.04012
H	-0.76474	-3.77234	2.48585	H	-3.91720	1.95090	-1.74672
H	-1.57476	-3.85925	0.90784	H	-4.11112	1.54319	-0.02871
H	5.92271	-1.93572	-0.14899	H	2.03013	5.72176	-0.67735
C	-2.90275	-3.48651	2.57867	C	-5.27631	0.31348	-1.38178
H	-3.12949	-4.54227	2.74160	H	-6.16424	0.94685	-1.33078
H	-2.88178	-2.98725	3.54888	H	-5.20219	-0.09229	-2.39194
H	-3.70979	-3.05187	1.98556	H	-5.40806	-0.51607	-0.68470
H	1.92596	1.84873	0.45858	H	2.48828	0.53916	-1.37540
O	2.86747	2.67943	0.60553	O	5.40936	-0.04433	-0.89823
O	2.14673	3.89124	-1.14784	O	4.90735	-1.10151	1.01832
C	2.98651	3.62663	-0.21331	C	5.74396	-0.47128	0.18701
C	4.16808	4.53716	-0.11031	C	7.13213	-0.35991	0.75703
H	4.93479	4.10157	0.52418	H	7.77992	0.16568	0.06081
H	4.56095	4.75196	-1.10362	H	7.09983	0.17184	1.70969
H	3.83559	5.48321	0.32461	H	7.53087	-1.35653	0.95530
TS9				TS9b			
C	-0.39937	-0.81382	-1.58698	C	-1.38266	-1.28737	-0.88680
C	1.11299	-1.17510	-1.60527	C	-0.34710	-2.31741	-0.48704
C	-0.77978	-0.08576	-2.87677	C	-1.03402	-0.70084	-2.27199
H	-0.38445	-0.60476	-3.75876	H	-1.11977	-1.53705	-2.98615

H	-1.85991	-0.01650	-2.99671	H	-1.73709	0.06675	-2.58201
H	-0.35920	0.91562	-2.89742	H	-0.01883	-0.32650	-2.34369
C	2.18044	-0.16014	-1.98529	C	0.96673	-1.65234	-0.14231
O	2.05659	0.60252	-2.92820	O	1.05347	-0.39385	-0.15369
C	3.51256	-0.25346	-1.28715	C	2.11922	-2.46376	0.23901
C	4.64018	0.21549	-1.97092	C	3.26107	-1.85436	0.79122
C	3.67598	-0.77406	0.00040	C	2.11669	-3.86141	0.08222
C	5.89867	0.15541	-1.39104	C	4.36023	-2.61278	1.15557
C	4.93534	-0.81946	0.58840	C	3.22321	-4.61473	0.44431
C	6.04924	-0.36138	-0.10642	C	4.34909	-3.99603	0.98049
H	4.51080	0.62264	-2.96534	H	3.26794	-0.78422	0.94413
H	2.82418	-1.12254	0.56761	H	1.25217	-4.36442	-0.32982
H	6.76384	0.51096	-1.93840	H	5.22928	-2.12806	1.58451
H	5.04422	-1.21371	1.59175	H	3.20665	-5.68975	0.31042
H	7.03112	-0.40663	0.35022	H	5.21036	-4.58772	1.26679
H	0.92892	0.23596	2.35717	H	2.47869	0.34760	-0.99950
H	1.39559	-1.66525	-0.68162	H	-0.68187	-2.90377	0.37172
Ru	-1.01393	0.43010	0.13282	Ru	-0.52122	1.11334	-0.01304
C	-1.95296	2.36333	1.08474	C	-0.48893	2.98752	1.29453
C	-2.20641	2.51855	-0.32109	C	0.68462	3.04095	0.52271
C	-2.85795	1.47872	-0.97436	C	0.54669	2.87971	-0.89061
C	-3.22068	0.28662	-0.28962	C	-0.71232	2.80909	-1.52734
C	-3.07371	0.19073	1.11243	C	-1.89270	2.74851	-0.75377
C	-2.45705	1.27537	1.79541	C	-1.74850	2.78213	0.66304
H	-1.40787	3.12877	1.62027	H	-0.44913	3.06680	2.37223
H	-3.05697	1.56372	-2.03413	H	1.44031	2.85566	-1.50065
H	-3.68445	-0.52367	-0.83580	H	-0.76382	2.73322	-2.60635
H	-2.30899	1.22158	2.86650	H	-2.63222	2.68029	1.28011
C	-1.89852	3.80741	-1.05898	C	2.06529	3.31250	1.09196
C	-0.51015	4.38871	-0.77959	C	2.23266	2.95575	2.56994
C	-3.00005	4.83782	-0.74717	C	2.44130	4.78654	0.84990
H	-1.95281	3.57562	-2.12671	H	2.76526	2.69831	0.51735
H	0.27375	3.67754	-1.03426	H	1.98082	1.91295	2.76484
H	-0.36520	5.28957	-1.37886	H	3.26937	3.11314	2.87395
H	-0.39186	4.67486	0.26827	H	1.60839	3.58272	3.21119
H	-3.99101	4.45271	-0.99461	H	2.37552	5.04882	-0.20745
H	-2.99625	5.10752	0.31199	H	1.77397	5.45198	1.40384
H	-2.83437	5.74883	-1.32570	H	3.46376	4.97904	1.18324
C	-3.59337	-0.99612	1.86739	C	-3.25160	2.68337	-1.39180
H	-4.57679	-0.76210	2.28515	H	-3.64749	3.69223	-1.54606
H	-3.69855	-1.86284	1.21635	H	-3.21229	2.19190	-2.36481
H	-2.93237	-1.26172	2.69162	H	-3.95985	2.14345	-0.76304
C	-1.64757	-4.13481	-0.12328	C	-5.02367	-1.35600	0.02513
C	-1.02476	-2.89747	-0.25563	C	-3.64468	-1.14640	0.03286

C	-1.14599	-2.13036	-1.43045	C	-2.81998	-1.71365	-0.93595
C	-1.92626	-2.67731	-2.45640	C	-3.38116	-2.52827	-1.91574
C	-2.57157	-3.90348	-2.31679	C	-4.75445	-2.76216	-1.91228
C	-2.43364	-4.64266	-1.14985	C	-5.57644	-2.16775	-0.95445
C	-0.18951	-2.42539	0.91513	C	-2.91554	-0.48928	1.12105
H	-1.50923	-4.69120	0.79538	H	-5.63651	-0.90051	0.79314
H	-2.03614	-2.14656	-3.39120	H	-2.76476	-2.98364	-2.68115
H	-2.92856	-5.59988	-1.03826	H	-6.64466	-2.34793	-0.97300
O	0.51100	-3.21598	1.55341	O	-3.41948	-0.11979	2.17866
N	-0.42959	-1.12837	1.14787	N	-1.53027	-0.48735	0.88229
O	0.82024	-0.77377	2.50284	O	-0.90983	-1.16137	2.05649
C	0.24957	-1.01993	3.80134	C	-0.20467	-0.28620	2.93880
H	-0.02145	-2.07307	3.81277	H	-0.91973	0.36276	3.45251
H	-0.65503	-0.41753	3.91897	H	0.46475	0.34450	2.34830
H	-3.17550	-4.28292	-3.13336	H	-5.18735	-3.40626	-2.66856
C	1.26457	-0.69745	4.88457	C	0.56003	-1.15117	3.92190
H	0.82583	-0.90328	5.86395	H	1.10625	-0.51517	4.62280
H	2.15918	-1.31118	4.77214	H	-0.11669	-1.78520	4.49778
H	1.55563	0.35379	4.85542	H	1.27882	-1.79000	3.40671
H	1.24304	-1.94771	-2.38136	H	-0.19404	-3.02419	-1.31404
O	0.88733	1.33773	-0.08217	O	2.73225	-0.32366	-3.23259
O	1.31823	1.67810	2.09525	O	3.28928	0.78201	-1.35907
C	1.54109	1.87001	0.87657	C	3.48283	0.41605	-2.63477
C	2.67465	2.79310	0.49011	C	4.72786	1.02849	-3.21403
H	3.60494	2.40467	0.90670	H	5.59851	0.69926	-2.64369
H	2.76891	2.88936	-0.58817	H	4.83648	0.73596	-4.25471
H	2.50218	3.77406	0.93677	H	4.68036	2.11587	-3.13451
INT10				INT11			
C	-0.29836	-0.97867	-1.49801	C	0.71652	1.49960	1.10848
C	1.20188	-1.34453	-1.30607	C	2.04498	0.97587	0.52644
C	-0.52042	-0.48290	-2.92991	C	0.81918	1.55906	2.63810
H	-0.08469	-1.17486	-3.66326	H	1.73927	2.07369	2.93762
H	-1.57636	-0.37993	-3.17497	H	-0.01329	2.10381	3.08364
H	-0.03506	0.47515	-3.08416	H	0.88027	0.56620	3.06594
C	2.33509	-0.43005	-1.73879	C	2.56866	-0.37995	0.96523
O	2.27488	0.31060	-2.70476	O	2.05950	-1.03200	1.85982
C	3.65544	-0.57458	-1.02005	C	3.81159	-0.88875	0.28840
C	4.81153	-0.17615	-1.70336	C	4.29189	-2.15208	0.65146
C	3.78436	-1.06499	0.28360	C	4.51369	-0.15271	-0.67192
C	6.05949	-0.27438	-1.10762	C	5.43890	-2.66922	0.06835
C	5.03458	-1.14721	0.88804	C	5.66640	-0.66843	-1.25278
C	6.17414	-0.75875	0.19376	C	6.13046	-1.92699	-0.88621
H	4.71065	0.20689	-2.71043	H	3.74865	-2.71695	1.39751
H	2.91431	-1.36393	0.85214	H	4.17104	0.82778	-0.97380

H	6.94509	0.02645	-1.65505	H	5.79721	-3.65042	0.35685
H	5.11498	-1.51718	1.90321	H	6.20139	-0.08636	-1.99370
H	7.14819	-0.83237	0.66319	H	7.02792	-2.32873	-1.34198
H	1.08567	0.81705	2.19217	H	-2.89836	-1.48263	-2.42893
H	1.37899	-1.67254	-0.28946	H	2.01241	0.98704	-0.56135
Ru	-1.08965	0.51555	-0.05357	Ru	-0.99439	0.15361	0.49787
C	-2.20862	2.32803	0.91062	C	-2.32044	-1.84783	0.82591
C	-1.92833	2.62893	-0.45705	C	-1.46187	-1.91535	1.96714
C	-2.37452	1.73681	-1.45206	C	-1.41367	-0.79613	2.78388
C	-3.03910	0.53443	-1.09386	C	-2.17131	0.36745	2.47920
C	-3.28519	0.20526	0.25568	C	-3.15108	0.35572	1.45835
C	-2.85735	1.13973	1.24847	C	-3.21701	-0.79110	0.64030
H	-1.87280	2.98644	1.69777	H	-2.33593	-2.66330	0.11746
H	-2.17599	1.95289	-2.49210	H	-0.75677	-0.78992	3.64334
H	-3.34198	-0.16112	-1.86473	H	-2.09151	1.23409	3.12110
H	-3.01842	0.90274	2.29184	H	-3.88851	-0.82000	-0.21000
C	-1.22650	3.90892	-0.88210	C	-0.68815	-3.17013	2.31282
C	-0.53450	4.66167	0.25609	C	0.00062	-3.82362	1.11081
C	-2.22937	4.83912	-1.59061	C	-1.62475	-4.16455	3.02409
H	-0.46542	3.61838	-1.61303	H	0.08929	-2.87113	3.02001
H	0.13757	4.02180	0.82716	H	0.66292	-3.11958	0.60982
H	0.05200	5.48688	-0.15076	H	0.59682	-4.67195	1.45188
H	-1.26029	5.09052	0.95152	H	-0.72117	-4.20475	0.38512
H	-2.68670	4.35953	-2.45669	H	-2.08174	-3.72214	3.91134
H	-3.02860	5.13865	-0.90794	H	-2.42623	-4.49430	2.35818
H	-1.72309	5.74359	-1.93377	H	-1.06258	-5.04723	3.33531
C	-4.03495	-1.03445	0.64502	C	-4.07798	1.51339	1.24258
H	-5.09247	-0.79743	0.79647	H	-5.06986	1.27145	1.63369
H	-3.96450	-1.79910	-0.12697	H	-3.71941	2.40658	1.75296
H	-3.64831	-1.45069	1.57527	H	-4.17836	1.73407	0.17990
C	-1.68586	-4.08059	0.28879	C	0.16699	4.40423	-1.37627
C	-1.04226	-2.86306	0.07029	C	0.11288	3.14409	-0.78132
C	-1.07933	-2.24549	-1.20030	C	0.56919	2.91567	0.52912
C	-1.81910	-2.90177	-2.19586	C	1.04600	4.03531	1.22267
C	-2.48874	-4.09810	-1.95953	C	1.07359	5.30096	0.64314
C	-2.41768	-4.70321	-0.71276	C	0.64888	5.49268	-0.66571
C	-0.35524	-2.27253	1.27101	C	-0.53843	2.04149	-1.53990
H	-1.60967	-4.52614	1.27242	H	-0.19632	4.51787	-2.39060
H	-1.86942	-2.48289	-3.19017	H	1.41578	3.93534	2.23228
H	-2.92371	-5.64180	-0.52059	H	0.67758	6.47625	-1.11854
O	0.17028	-3.01132	2.12275	O	-0.39417	1.83974	-2.74355
N	-0.43777	-0.93355	1.34965	N	-1.43672	1.37011	-0.76333
O	0.24115	-0.43965	2.51752	O	-3.86334	-1.40053	-2.53922
C	-0.56559	-0.50925	3.71319	C	-4.12437	-0.47329	-3.59267

H	-0.90447	-1.53816	3.82709	H	-3.59612	0.46917	-3.40685
H	-1.43059	0.14739	3.59678	H	-5.19517	-0.26093	-3.54890
H	-3.05125	-4.56185	-2.76229	H	1.43898	6.14058	1.22352
C	0.29723	-0.08145	4.88187	C	-3.75429	-1.01825	-4.96443
H	-0.28767	-0.13371	5.80224	H	-4.00562	-0.29491	-5.74503
H	1.16143	-0.73873	4.98686	H	-2.68278	-1.22222	-5.02503
H	0.64989	0.94539	4.76612	H	-4.29178	-1.94668	-5.16873
H	1.39334	-2.24297	-1.91924	H	2.82948	1.69777	0.80220
O	0.93554	1.41068	-0.10424	O	0.40045	-0.78448	-0.71989
O	1.76031	1.54823	1.98160	O	-1.10437	-1.79538	-2.06348
C	1.75822	1.84247	0.70556	C	0.04876	-1.50422	-1.74258
C	2.86074	2.76778	0.28851	C	1.22420	-1.97938	-2.57372
H	2.76108	3.02794	-0.76100	H	2.08447	-2.21510	-1.94939
H	2.83879	3.66659	0.90701	H	0.93546	-2.84200	-3.17083
H	3.82078	2.27746	0.45841	H	1.51441	-1.16997	-3.24852
TS10				INT12			
C	0.06691	1.53600	-1.17596	C	-1.21996	2.00244	-0.69204
C	-1.40199	1.86232	-0.87317	C	-2.12307	1.45803	0.44425
C	0.24668	1.15030	-2.62752	C	-1.90031	1.83452	-2.06224
H	-0.23123	1.91099	-3.25674	H	-2.87617	2.32551	-2.07087
H	1.29073	1.08516	-2.91354	H	-1.28304	2.28560	-2.83953
H	-0.25995	0.21753	-2.85059	H	-2.04213	0.78177	-2.30662
C	-2.50723	0.89378	-1.29310	C	-2.54313	0.02607	0.26971
O	-2.63337	0.55493	-2.45648	O	-1.77117	-0.80740	-0.22104
C	-3.54556	0.53632	-0.28288	C	-3.88992	-0.43293	0.67827
C	-4.83571	0.24982	-0.73724	C	-4.28336	-1.74226	0.36109
C	-3.26543	0.45635	1.08319	C	-4.77597	0.38737	1.38913
C	-5.83474	-0.09991	0.15873	C	-5.53098	-2.21151	0.73417
C	-4.26359	0.09045	1.97666	C	-6.02162	-0.09130	1.77271
C	-5.54895	-0.18243	1.51896	C	-6.40340	-1.38681	1.44250
H	-5.03994	0.30582	-1.79857	H	-3.59881	-2.37883	-0.18209
H	-2.25596	0.62361	1.43346	H	-4.49935	1.39666	1.66117
H	-6.83498	-0.31051	-0.20019	H	-5.82765	-3.22110	0.47669
H	-4.03733	0.01207	3.03238	H	-6.69506	0.54950	2.32856
H	-6.32642	-0.46101	2.22044	H	-7.37895	-1.75548	1.73672
H	-0.08530	-2.74202	2.34999	H	4.14052	-0.77192	1.35270
H	-1.53037	2.15970	0.15833	H	-1.56410	1.50991	1.38328
Ru	0.99359	-0.46090	0.01413	Ru	0.33377	-0.71912	-0.66643
C	2.08433	-2.42864	-0.58170	C	1.87695	-2.32441	-0.63677
C	2.32328	-1.49755	-1.61156	C	0.66890	-2.93588	-1.02702
C	2.86123	-0.24090	-1.22765	C	-0.02335	-2.32565	-2.11064
C	3.18283	0.08169	0.11057	C	0.49870	-1.22438	-2.82732
C	2.89466	-0.84194	1.13356	C	1.73169	-0.64375	-2.43675
C	2.33586	-2.10496	0.75826	C	2.39733	-1.18387	-1.30790

H	1.61132	-3.37437	-0.80035	H	2.38490	-2.65492	0.25504
H	3.03029	0.51019	-1.98740	H	-1.01305	-2.68541	-2.36612
H	3.58922	1.05489	0.34923	H	-0.07011	-0.79809	-3.64169
H	2.04374	-2.79264	1.53682	H	3.29138	-0.71392	-0.92672
C	2.08585	-1.83547	-3.06526	C	0.07938	-4.15550	-0.34792
C	0.79819	-2.62864	-3.30101	C	0.48206	-4.30945	1.12021
C	3.30968	-2.58142	-3.62062	C	0.43281	-5.42011	-1.14992
H	2.00393	-0.88988	-3.60492	H	-1.00817	-4.03169	-0.38366
H	-0.06532	-2.12936	-2.86143	H	0.25060	-3.41249	1.69545
H	0.62578	-2.74113	-4.37243	H	-0.05783	-5.14837	1.56319
H	0.86178	-3.63262	-2.87609	H	1.54899	-4.51808	1.22748
H	4.22392	-1.99897	-3.49246	H	0.10718	-5.34221	-2.18917
H	3.44340	-3.53852	-3.11081	H	1.51240	-5.59083	-1.14697
H	3.17842	-2.78050	-4.68580	H	-0.04862	-6.29584	-0.70968
C	3.15390	-0.53883	2.57520	C	2.29321	0.53193	-3.17510
H	2.43785	-1.06601	3.20351	H	2.99122	0.17265	-3.93761
H	4.16008	-0.87760	2.83863	H	1.50689	1.09470	-3.67745
H	3.08515	0.52864	2.77748	H	2.82342	1.19418	-2.49409
C	1.82767	3.94539	1.17832	C	1.02070	4.85690	-0.03861
C	1.13444	2.83652	0.70983	C	0.44541	3.61713	-0.27957
C	0.95671	2.62348	-0.66988	C	-0.92312	3.46886	-0.42845
C	1.56130	3.52226	-1.55343	C	-1.76746	4.56701	-0.34871
C	2.27878	4.61601	-1.07991	C	-1.20009	5.81816	-0.10661
C	2.40387	4.84008	0.28588	C	0.18035	5.96335	0.04759
C	0.66489	1.81176	1.70205	C	1.08521	2.27552	-0.41651
H	1.93736	4.06931	2.24801	H	2.09407	4.95186	0.07661
H	1.45126	3.39123	-2.62080	H	-2.84105	4.47225	-0.46945
H	2.96123	5.69328	0.65220	H	0.59591	6.94644	0.23532
O	0.77121	1.97468	2.92287	O	2.30314	2.07023	-0.31196
N	0.09584	0.72596	1.14522	N	0.10980	1.37510	-0.66370
O	0.30821	-2.61808	3.23842	O	5.02953	-0.76102	0.95064
C	-0.42809	-1.59673	3.90693	C	5.69671	0.42877	1.36455
H	-0.40708	-0.67102	3.32114	H	5.08692	1.30807	1.12514
H	0.10290	-1.39973	4.84141	H	6.60666	0.49124	0.76261
H	2.73183	5.30098	-1.78661	H	-1.83944	6.69062	-0.03737
C	-1.86377	-2.00678	4.19562	C	6.04932	0.42427	2.84544
H	-2.38632	-1.21652	4.74175	H	6.58934	1.33621	3.11540
H	-2.40680	-2.19276	3.26661	H	5.14627	0.37094	3.45788
H	-1.89244	-2.91803	4.79684	H	6.67900	-0.43396	3.09006
H	-1.61400	2.75237	-1.48502	H	-2.99738	2.09796	0.54017
O	-0.91760	-1.18405	-0.44450	O	0.34361	-0.42296	1.42457
O	-0.75862	-3.09430	0.73184	O	2.45320	-0.95187	2.01810
C	-1.34660	-2.33066	-0.04772	C	1.30341	-0.56879	2.26776
C	-2.69885	-2.72452	-0.60489	C	0.93132	-0.19766	3.69594

H	-2.91588	-2.20524	-1.53528	H	1.51383	-0.78833	4.40129
H	-2.73736	-3.80376	-0.74536	H	1.17811	0.85562	3.85319
H	-3.46491	-2.45070	0.12369	H	-0.13401	-0.32671	3.87983
TS11				INT13			
C	1.43658	-0.80883	-1.76259	C	1.44738	-0.22252	-1.90278
C	1.93130	0.58770	-1.35480	C	1.48845	1.23841	-1.41816
C	1.17623	-0.94911	-3.26940	C	0.99797	-0.35451	-3.37478
H	2.08080	-0.70110	-3.82852	H	1.64534	0.25411	-4.01020
H	0.90712	-1.98021	-3.50172	H	1.09220	-1.39177	-3.69876
H	0.38622	-0.27918	-3.59048	H	-0.01862	-0.00944	-3.51280
C	1.05458	1.78327	-1.67158	C	0.34726	2.19059	-1.73796
O	0.13787	1.73479	-2.47432	O	-0.61303	1.88917	-2.42430
C	1.40014	3.07706	-1.00410	C	0.47439	3.59699	-1.21891
C	0.62581	4.20280	-1.30478	C	-0.53671	4.51097	-1.53702
C	2.45996	3.20303	-0.10110	C	1.55621	4.03277	-0.44667
C	0.89963	5.42617	-0.71540	C	-0.47086	5.82354	-1.09582
C	2.73740	4.43294	0.48383	C	1.62336	5.34942	-0.00528
C	1.96031	5.54430	0.18080	C	0.61170	6.24678	-0.32771
H	-0.19254	4.09632	-2.00424	H	-1.37125	4.17146	-2.13620
H	3.06125	2.34899	0.17908	H	2.35218	3.35175	-0.17817
H	0.29034	6.29016	-0.95218	H	-1.26144	6.51991	-1.34970
H	3.55724	4.51776	1.18665	H	2.46665	5.67294	0.59313
H	2.17626	6.50043	0.64270	H	0.66517	7.27263	0.01781
H	2.14087	0.56840	-0.28784	H	1.72246	0.75318	3.38217
Ru	-1.63648	-0.50751	-0.33363	H	1.64108	1.22807	-0.33808
C	-3.83799	-0.47956	0.06023	Ru	-1.35856	-0.96986	-0.23143
C	-3.47119	0.78869	-0.40088	C	-3.38467	-1.75313	0.28494
C	-2.69896	0.84877	-1.60552	C	-3.55939	-0.44868	-0.19013
C	-2.38090	-0.32057	-2.33856	C	-2.95486	-0.13380	-1.45322
C	-2.78021	-1.61145	-1.88299	C	-2.28988	-1.11035	-2.21540
C	-3.46005	-1.66100	-0.65137	C	-2.13827	-2.44907	-1.73473
H	-4.28492	-0.59209	1.03475	C	-2.65828	-2.73475	-0.46181
H	-2.28924	1.79278	-1.93335	H	-3.70691	-2.00973	1.28322
H	-1.75265	-0.23011	-3.21088	H	-2.96082	0.88731	-1.80867
H	-3.64977	-2.62260	-0.19425	H	-1.83795	-0.82562	-3.15209
C	-3.72699	2.06691	0.35801	H	-2.47427	-3.70321	-0.01664
C	-4.00733	1.85929	1.84426	C	-4.26696	0.64392	0.57913
C	-4.85837	2.84995	-0.32582	C	-4.38953	0.37584	2.07914
H	-2.80427	2.64819	0.27275	C	-5.64603	0.90851	-0.05079
H	-3.22383	1.26352	2.31156	H	-3.65451	1.54143	0.44973
H	-4.05818	2.82765	2.34491	H	-3.41713	0.16747	2.52701
H	-4.96615	1.35960	2.00594	H	-4.81134	1.25190	2.57470
H	-4.64081	3.03824	-1.37889	H	-5.05535	-0.46567	2.28774
H	-5.79989	2.29833	-0.26817	H	-5.56777	1.14524	-1.11364

H	-4.99965	3.81319	0.16769	H	-6.29510	0.03545	0.05408
C	-2.38626	-2.85473	-2.61690	H	-6.13024	1.75124	0.44635
H	-3.13369	-3.09661	-3.37724	C	-1.41756	-3.48699	-2.53886
H	-1.42692	-2.72382	-3.11531	H	-2.12771	-3.99802	-3.19575
H	-2.30762	-3.69863	-1.93268	H	-0.64822	-3.03760	-3.16457
C	2.60071	-3.79231	0.10452	H	-0.94916	-4.22646	-1.89171
C	1.89171	-2.73078	-0.43862	C	3.86618	-2.86727	-0.99983
C	2.47323	-1.84458	-1.33925	C	2.76249	-2.04048	-1.16154
C	3.79273	-2.00486	-1.72698	C	2.84244	-0.83196	-1.83205
C	4.51700	-3.06601	-1.18340	C	4.04776	-0.40926	-2.37274
C	3.92954	-3.95110	-0.27793	C	5.16763	-1.22459	-2.20843
C	0.50462	-2.27983	-0.23547	C	5.07997	-2.44310	-1.53143
H	2.13247	-4.46995	0.80810	C	1.37374	-2.19638	-0.68560
H	4.26503	-1.32565	-2.42722	H	3.77870	-3.80894	-0.47129
H	4.51643	-4.76465	0.13059	H	4.13548	0.52845	-2.91020
O	-0.38486	-2.79485	0.50961	H	5.96548	-3.05738	-1.41940
N	0.26042	-1.21323	-0.96544	O	0.96485	-3.22194	-0.05770
H	5.55414	-3.20325	-1.46501	N	0.65365	-1.13104	-1.00847
H	2.89339	0.77847	-1.84441	O	2.10940	0.63228	4.27690
O	-0.68804	1.05625	0.68700	C	3.39130	0.02826	4.13815
O	0.92759	0.00425	1.84125	H	3.32946	-0.85562	3.49121
C	0.20416	0.98294	1.60876	H	3.67645	-0.32114	5.13403
C	0.30354	2.23263	2.46196	H	6.12181	-0.90763	-2.61328
H	1.27867	2.29914	2.94033	C	4.44590	0.98838	3.60444
H	0.11027	3.12606	1.87187	H	5.42263	0.49889	3.55342
H	-0.46270	2.16748	3.23906	H	4.18639	1.33123	2.60018
H	-0.40989	-2.64226	2.03495	H	4.53260	1.86320	4.25257
O	-0.54039	-2.52907	3.03756	H	2.38233	1.70608	-1.84448
O	-1.98375	-0.95621	2.35156	O	-0.95869	0.96049	0.58201
C	-1.39449	-1.54678	3.24501	O	0.93859	0.75739	1.77659
C	-1.57082	-1.20334	4.69839	C	-0.14753	1.29903	1.52143
H	-1.66882	-2.10721	5.29962	C	-0.62403	2.47740	2.35490
H	-0.67677	-0.67605	5.03972	H	0.21037	2.94995	2.86981
H	-2.43735	-0.56083	4.83086	H	-1.14785	3.20518	1.73712
C	5.70262	-0.25995	1.21631	H	-1.32915	2.10614	3.10330
H	6.31033	-1.16454	1.14499	H	0.71136	-3.12439	1.32679
H	5.58125	0.15068	0.21193	O	0.58394	-3.07520	2.37078
H	6.24180	0.47076	1.82349	O	-0.89397	-1.45603	1.88548
C	4.35282	-0.57440	1.82847	C	-0.26002	-2.14212	2.69381
H	4.48906	-1.03107	2.81807	C	-0.41528	-1.90523	4.16725
H	3.81932	-1.29737	1.20553	H	0.33975	-1.17002	4.46467
O	3.59709	0.62990	1.94367	H	-1.39968	-1.49563	4.38274
H	2.65121	0.38873	2.03514	H	-0.24693	-2.82270	4.72861
TS12							

C	-0.94878	0.92427	-1.23335
C	-1.80793	0.40627	-0.03778
C	-1.31470	0.27762	-2.56856
H	-2.36446	0.44376	-2.80187
H	-0.70522	0.69922	-3.36935
H	-1.14895	-0.79868	-2.54294
C	-3.29194	0.73748	-0.07844
O	-3.98981	0.25192	-0.95729
C	-3.90711	1.59924	0.97694
C	-5.30413	1.71560	0.99612
C	-3.16059	2.29344	1.93583
C	-5.93600	2.49942	1.94731
C	-3.79510	3.08557	2.88536
C	-5.18131	3.18815	2.89539
H	-5.87891	1.17842	0.25335
H	-2.08103	2.23595	1.94566
H	-7.01678	2.57661	1.95360
H	-3.20451	3.62238	3.61787
H	-5.67434	3.80279	3.63943
H	-1.75630	-0.67802	-0.02388
H	-1.33617	0.75714	0.87630
Ru	1.36485	-1.30240	-0.14149
C	1.33270	-3.09545	1.12806
C	-0.03200	-2.84080	0.80711
C	-0.34100	-2.70976	-0.56399
C	0.62688	-2.87655	-1.58762
C	1.95958	-3.17703	-1.25076
C	2.30439	-3.27353	0.12925
H	1.65997	-3.09056	2.15623
H	-1.35834	-2.47652	-0.85125
H	0.34631	-2.75282	-2.62460
H	3.33743	-3.39919	0.41783
C	-1.11872	-2.80047	1.86207
C	-0.71595	-2.07269	3.14808
C	-1.58269	-4.23811	2.16085
H	-1.96978	-2.26911	1.42739
H	-0.34572	-1.06923	2.93831
H	-1.57966	-1.99482	3.81081
H	0.06124	-2.61460	3.69172
H	-1.92321	-4.74611	1.25654
H	-0.77127	-4.82740	2.59525
H	-2.40872	-4.22497	2.87468
C	3.00546	-3.36000	-2.30693
H	2.73005	-2.85719	-3.23350

H	3.97297	-2.98922	-1.97138	
H	3.11293	-4.42749	-2.52113	
C	0.24781	4.37681	-0.65231	
C	0.08810	3.00139	-0.77523	
C	-1.06943	2.43812	-1.27858	
C	-2.11505	3.24913	-1.70408	
C	-1.96600	4.62936	-1.58932	
C	-0.80041	5.19148	-1.06025	
C	1.07800	1.92985	-0.52815	
H	1.17021	4.79083	-0.26294	
H	-3.02542	2.83503	-2.11976	
H	-0.71356	6.26863	-0.98270	
O	2.23473	2.11771	-0.19959	
N	0.50221	0.69105	-0.90321	
H	-2.76777	5.27996	-1.91880	
O	1.72494	-0.10775	1.52629	
O	3.44610	-1.26701	2.41304	
C	2.66627	-0.31173	2.38874	
C	2.74271	0.78367	3.44265	
H	3.54300	0.57575	4.14969	
H	2.91817	1.74462	2.95656	
H	1.79309	0.85761	3.97600	
H	1.28154	0.45594	-1.96883	
O	2.17669	0.40052	-2.74257	
O	3.18924	-0.50238	-0.96706	
C	3.22491	0.08403	-2.07259	
C	4.55174	0.45845	-2.66613	
H	5.36795	-0.02763	-2.13808	
H	4.57192	0.19891	-3.72485	
H	4.66676	1.54191	-2.58972	
TS21				INT21
Ru	1.25535	0.65317	0.28318	Ru -1.19198 0.78305 -0.36389
C	2.46821	0.20151	2.26121	C -2.51349 0.62364 -2.28896
C	2.98510	-0.63073	1.26173	C -3.09088 -0.20644 -1.31570
C	3.36538	0.00194	0.03689	C -3.32759 0.37360 -0.03578
C	3.30451	1.40437	-0.12429	C -3.08090 1.75137 0.20766
C	2.84289	2.25362	0.92203	C -2.56007 2.60595 -0.79539
C	2.37737	1.61315	2.07891	C -2.20498 1.98441 -2.00892
H	2.11031	-0.22129	3.18899	H -2.26402 0.22818 -3.26397
H	3.72427	-0.60579	-0.78425	H -3.73752 -0.23649 0.75923
H	3.61294	1.84158	-1.06509	H -3.28447 2.15433 1.19234
H	1.92630	2.20852	2.86332	H -1.70899 2.57120 -2.77289
C	3.22499	-2.11513	1.44629	C -3.54488 -1.62403 -1.60006
C	2.24996	-2.79286	2.41108	C -2.65469 -2.38263 -2.58716

C	4.68211	-2.35363	1.88362	C	-5.00790	-1.61512	-2.07967
H	3.10075	-2.57440	0.46083	H	-3.51926	-2.15683	-0.64485
H	1.21237	-2.59843	2.13447	H	-1.60937	-2.36741	-2.27393
H	2.41014	-3.87257	2.40428	H	-2.97558	-3.42380	-2.65670
H	2.39807	-2.45185	3.43852	H	-2.71425	-1.95891	-3.59239
H	5.38965	-1.91265	1.17902	H	-5.66014	-1.11408	-1.36199
H	4.86776	-1.91575	2.86757	H	-5.09876	-1.09639	-3.03735
H	4.88895	-3.42426	1.94495	H	-5.37163	-2.63654	-2.21246
C	2.84304	3.74733	0.77874	C	-2.36276	4.07613	-0.56408
H	2.08821	4.20135	1.42118	H	-1.54157	4.46116	-1.16997
H	3.81642	4.16070	1.05963	H	-3.26444	4.63645	-0.83083
H	2.64089	4.04454	-0.25084	H	-2.14066	4.28436	0.48330
O	-4.13920	-1.89286	-0.03089	O	4.36850	-1.83856	-0.16254
C	-4.65719	-1.74828	1.06808	C	4.95152	-1.56719	-1.19630
O	-4.42709	-0.72962	1.87201	O	4.68430	-0.49736	-1.93955
C	-5.63867	-2.73558	1.64082	C	6.05891	-2.40355	-1.77406
H	-5.26947	-3.11063	2.59702	H	5.79417	-2.72043	-2.78441
H	-6.59016	-2.23688	1.83438	H	6.96934	-1.80617	-1.84983
H	-5.78766	-3.56171	0.95096	H	6.23688	-3.27244	-1.14671
C	-2.40618	3.59972	-0.46525	C	2.54307	3.42321	1.00162
C	-1.61052	2.45566	-0.49844	C	1.74383	2.29151	0.83765
C	-0.58943	2.31444	-1.46385	C	0.66460	2.00538	1.70238
C	-0.41069	3.38159	-2.36089	C	0.44047	2.92077	2.74520
C	-1.18839	4.52972	-2.29929	C	1.22527	4.05619	2.89254
C	-2.19864	4.64636	-1.35173	C	2.28499	4.31921	2.02566
C	-1.89996	1.40669	0.50998	C	2.03796	1.37722	-0.25816
H	-3.19307	3.65350	0.27578	H	3.36094	3.58647	0.31164
H	0.35039	3.31868	-3.12455	H	-0.35670	2.74687	3.45318
H	-2.81649	5.53467	-1.30583	H	2.89771	5.20259	2.15284
O	-3.06400	1.25704	0.94385	O	3.03658	1.43738	-0.96040
N	-0.83277	0.70086	0.94016	N	1.02579	0.40097	-0.51780
O	-1.20246	-0.33473	1.83315	O	1.46397	-0.52329	-1.49860
C	-1.15608	0.12931	3.19500	C	1.09649	-0.10611	-2.82977
H	-1.88827	0.93023	3.32517	H	1.60710	0.82940	-3.06971
H	-0.16098	0.53249	3.40011	H	0.01880	0.06132	-2.84096
H	-3.78345	-0.05068	1.47662	H	3.96657	0.05570	-1.53696
H	-1.01126	5.33012	-3.00881	H	1.01364	4.74162	3.70580
C	-1.47028	-1.04900	4.09179	C	1.50529	-1.21553	-3.77355
H	-1.43880	-0.73189	5.13620	H	1.22964	-0.93891	-4.79312
H	-2.46664	-1.43943	3.88222	H	2.58287	-1.38050	-3.74557
H	-0.74364	-1.85166	3.95570	H	1.00006	-2.14990	-3.52403
C	0.25586	1.10468	-1.57300	C	-0.13846	0.78811	1.52920
C	-0.02331	-0.12792	-0.89180	C	0.29157	-0.25347	0.59536
C	1.05663	0.95133	-2.86308	C	-0.96452	0.37760	2.73484

H	0.40965	1.00728	-3.74372	H	-0.34412	0.22304	3.62408
H	1.81174	1.73508	-2.95474	H	-1.69734	1.14890	2.98095
H	1.57457	-0.00544	-2.88754	H	-1.51356	-0.53970	2.54708
C	-0.93371	-1.28317	-1.14681	C	0.83964	-1.64236	0.92757
O	-2.17056	-0.84741	-1.68331	O	2.12205	-1.48566	1.54685
C	-0.21177	-2.24906	-2.09131	C	-0.04974	-2.51531	1.79199
C	0.74875	-3.12849	-1.59306	C	-1.22584	-3.04365	1.25824
C	-0.51468	-2.27039	-3.45052	C	0.30289	-2.85230	3.09673
C	1.40070	-4.01617	-2.44045	C	-2.04654	-3.86820	2.01793
C	0.13839	-3.15827	-4.29991	C	-0.51728	-3.67819	3.86050
C	1.09851	-4.03126	-3.79929	C	-1.69635	-4.18652	3.32730
H	0.97799	-3.12346	-0.53472	H	-1.49866	-2.80215	0.23937
H	-1.27331	-1.60158	-3.83425	H	1.22427	-2.46613	3.50998
H	2.13778	-4.70206	-2.03928	H	-2.95541	-4.27068	1.58517
H	-0.10803	-3.17031	-5.35535	H	-0.22936	-3.92830	4.87532
H	1.60312	-4.72485	-4.46154	H	-2.33239	-4.83215	3.92149
H	-2.88198	-1.13041	-1.07473	H	2.81726	-1.55204	0.86939
H	-1.09130	-1.79788	-0.19541	H	0.96447	-2.16488	-0.02156
TS22				INT22			
Ru	0.93782	-0.94840	-0.10718	Ru	1.08973	-0.80834	-0.97723
C	2.41363	-1.70469	-1.74252	C	2.64235	-1.82887	-2.18031
C	3.18754	-0.94946	-0.83866	C	2.12218	-0.80255	-2.98791
C	3.07512	-1.28481	0.53220	C	2.10266	0.51919	-2.43646
C	2.29292	-2.38717	0.96627	C	2.62076	0.79338	-1.16329
C	1.55917	-3.17907	0.05761	C	3.16675	-0.25360	-0.35535
C	1.58369	-2.76431	-1.29624	C	3.15411	-1.56156	-0.87714
H	2.41596	-1.46037	-2.79530	H	2.59454	-2.85625	-2.51250
H	3.61035	-0.69729	1.26722	H	1.60689	1.30805	-2.98585
H	2.23825	-2.60706	2.02549	H	2.55460	1.79886	-0.76823
H	0.97522	-3.29234	-2.01964	H	3.49640	-2.38422	-0.26411
C	4.15780	0.13306	-1.27089	C	1.58905	-1.02594	-4.38834
C	3.79518	0.81133	-2.59364	C	1.17517	-2.46816	-4.68470
C	5.58414	-0.44389	-1.33229	C	2.63497	-0.53878	-5.40848
H	4.14264	0.89421	-0.48455	H	0.70712	-0.38603	-4.48942
H	2.76993	1.18483	-2.59016	H	0.46387	-2.84924	-3.95033
H	4.46296	1.65573	-2.77276	H	0.70275	-2.51881	-5.66690
H	3.90415	0.12877	-3.43987	H	2.03748	-3.13899	-4.70576
H	5.88107	-0.88140	-0.37764	H	2.90349	0.50623	-5.24405
H	5.65552	-1.22122	-2.09731	H	3.54702	-1.13752	-5.34539
H	6.29998	0.34217	-1.58199	H	2.23941	-0.62927	-6.42178
C	0.77895	-4.38171	0.49956	C	3.72893	0.03052	1.00329
H	-0.09872	-4.53345	-0.12970	H	3.66918	-0.84659	1.64685
H	1.39576	-5.28308	0.43371	H	4.78335	0.30583	0.90562
H	0.44867	-4.27837	1.53344	H	3.21414	0.85776	1.48903

O	-4.21644	2.02213	-0.89086	O	-0.85514	3.26782	-1.35179
C	-4.73532	1.40448	-1.80719	C	-0.94694	2.97051	-2.56265
O	-4.09548	0.52052	-2.55655	O	-0.90497	1.79293	-3.04610
C	-6.17820	1.56732	-2.20073	C	-1.14352	4.09626	-3.56967
H	-6.65618	2.31519	-1.57399	H	-0.59669	3.89290	-4.49043
H	-6.24477	1.86086	-3.24978	H	-2.20494	4.15485	-3.82530
H	-6.69534	0.61142	-2.09820	H	-0.83767	5.05336	-3.15085
C	-3.03863	-2.25563	1.97376	C	-1.79118	-3.70521	1.69692
C	-2.02283	-1.46839	1.44718	C	-1.35201	-2.36865	1.74041
C	-1.02889	-0.89929	2.26744	C	-1.86437	-1.45737	2.70188
C	-1.09518	-1.17384	3.63521	C	-2.81826	-1.95770	3.62151
C	-2.10829	-1.97451	4.16149	C	-3.23041	-3.26969	3.57205
C	-3.08854	-2.51323	3.33975	C	-2.72083	-4.15465	2.60398
C	-1.96712	-1.25985	-0.02039	C	-0.38312	-1.86319	0.82431
H	-3.77876	-2.67054	1.30171	H	-1.38003	-4.36577	0.94382
H	-0.35757	-0.76128	4.30848	H	-3.23072	-1.30225	4.37599
H	-3.87636	-3.13176	3.75128	H	-3.05966	-5.18302	2.57892
O	-2.65671	-1.84845	-0.82097	O	0.13092	-2.51919	-0.17314
N	-0.94305	-0.34952	-0.41789	N	0.05724	-0.60926	0.90488
O	-1.54289	0.42178	-1.94016	O	-0.88424	-0.30608	-1.68180
C	-0.58310	0.25067	-2.93669	C	-1.73142	-1.23527	-2.38225
H	0.38200	0.02794	-2.43909	H	-1.55490	-2.21753	-1.94708
H	-0.44216	1.21541	-3.44338	H	-1.43644	-1.26998	-3.43546
H	-3.13393	0.42905	-2.26804	H	-0.89038	0.61161	-2.18619
H	-2.12737	-2.17056	5.22749	H	-3.96069	-3.62686	4.28916
C	-0.91713	-0.85240	-3.93191	C	-3.19028	-0.83787	-2.25069
H	-0.12038	-0.94685	-4.67485	H	-3.81876	-1.55810	-2.78062
H	-1.03176	-1.80898	-3.41959	H	-3.49371	-0.82058	-1.20272
H	-1.84816	-0.63731	-4.45998	H	-3.36660	0.14961	-2.67996
C	0.00793	-0.00952	1.67594	C	-1.42540	-0.08883	2.70124
C	-0.31465	0.62776	0.42521	C	-0.47154	0.29400	1.78706
C	0.95975	0.64026	2.65672	C	-2.02870	0.87824	3.68587
H	0.42962	1.27299	3.37502	H	-3.11874	0.88410	3.60242
H	1.49608	-0.12026	3.22865	H	-1.78406	0.60424	4.71647
H	1.69506	1.25730	2.15022	H	-1.68720	1.89328	3.51596
C	-0.54596	2.10202	0.10118	C	0.04442	1.72027	1.62728
O	-1.84461	2.46652	0.56811	O	-1.00475	2.60083	1.25424
C	0.47830	3.06013	0.67603	C	0.80279	2.26847	2.83383
C	1.73764	3.15955	0.08296	C	1.48746	1.43125	3.71628
C	0.18237	3.88214	1.76126	C	0.88118	3.64861	3.02790
C	2.69171	4.04001	0.57894	C	2.23025	1.95896	4.76806
C	1.13531	4.76585	2.25943	C	1.62080	4.17746	4.08017
C	2.39434	4.84547	1.67465	C	2.29945	3.33507	4.95511
H	1.97033	2.54178	-0.77565	H	1.43353	0.35622	3.59288

H	-0.79915	3.82911	2.21191	H	0.34646	4.30254	2.35206
H	3.66375	4.10565	0.10368	H	2.75013	1.29122	5.44546
H	0.88988	5.39755	3.10556	H	1.66551	5.25192	4.21732
H	3.13439	5.53632	2.06124	H	2.87360	3.74692	5.77674
H	-2.52023	2.17204	-0.07113	H	-0.98269	2.71538	0.27608
H	-0.51164	2.19925	-0.98299	H	0.76093	1.67203	0.80140
TS23				INT23			
Ru	1.28356	-0.25741	-0.67458	Ru	0.51723	-0.74801	-1.05554
C	3.04126	-0.62652	-1.99447	C	1.59700	-0.73424	-2.98800
C	3.28222	-1.36548	-0.82809	C	1.91337	0.47785	-2.31704
C	2.23327	-2.22553	-0.36368	C	2.41309	0.35993	-0.99290
C	1.04713	-2.40505	-1.09093	C	2.62062	-0.89462	-0.36789
C	0.79708	-1.64717	-2.27314	C	2.28922	-2.08635	-1.05312
C	1.80191	-0.72990	-2.68957	C	1.78254	-1.99172	-2.38150
H	3.75099	0.12010	-2.31858	H	1.11218	-0.70481	-3.95287
H	2.34147	-2.71545	0.59367	H	2.59632	1.26219	-0.42213
H	0.27593	-3.05331	-0.69640	H	2.96429	-0.93625	0.65615
H	1.61327	-0.08186	-3.53386	H	1.45483	-2.88701	-2.88925
C	4.57413	-1.29499	-0.03908	C	1.77875	1.84334	-2.96100
C	5.48920	-0.13310	-0.42423	C	0.60145	1.96417	-3.93229
C	5.31491	-2.63922	-0.18157	C	3.10306	2.22030	-3.64829
H	4.29109	-1.17412	1.01037	H	1.61329	2.55665	-2.14708
H	4.97063	0.81967	-0.32753	H	-0.33600	1.66830	-3.46022
H	6.35648	-0.11919	0.23828	H	0.50728	2.99845	-4.26795
H	5.86406	-0.23729	-1.44627	H	0.74637	1.34803	-4.82282
H	4.70109	-3.48262	0.13948	H	3.94152	2.18818	-2.94986
H	5.61220	-2.81243	-1.21900	H	3.32225	1.53493	-4.47106
H	6.21819	-2.63007	0.43116	H	3.04198	3.23041	-4.05837
C	-0.47606	-1.79660	-3.04734	C	2.41349	-3.42323	-0.38940
H	-0.76285	-0.85730	-3.51984	H	1.64259	-4.10518	-0.74663
H	-0.33400	-2.54011	-3.83722	H	3.38840	-3.85838	-0.62886
H	-1.29453	-2.13555	-2.41406	H	2.33716	-3.33532	0.69371
O	0.84386	-0.53754	1.81952	O	-1.35719	-0.39800	-1.95022
C	1.62340	-0.58275	2.82795	C	-1.85941	-1.07175	-2.92496
O	2.78299	-0.11254	2.86092	O	-1.32280	-2.01838	-3.51656
C	1.07454	-1.25783	4.07850	C	-3.25410	-0.62878	-3.33521
H	0.70189	-2.25482	3.83675	H	-3.40487	-0.80625	-4.39890
H	1.83920	-1.32649	4.84921	H	-3.98240	-1.23197	-2.78693
H	0.22977	-0.68100	4.46223	H	-3.43149	0.41771	-3.09372
C	-0.97892	4.11799	-1.08298	C	-2.65476	-2.45153	2.26975
C	-1.30043	2.83040	-0.61883	C	-2.07849	-1.21047	1.94390
C	-2.53721	2.57008	0.02655	C	-2.45579	-0.02391	2.62653
C	-3.43314	3.65736	0.16737	C	-3.42307	-0.14833	3.65295
C	-3.10844	4.91050	-0.30178	C	-3.97441	-1.37098	3.96342

C	-1.87391	5.15122	-0.92995	C	-3.59491	-2.53418	3.26995
C	-0.39129	1.73226	-0.75635	C	-1.08758	-1.08827	0.92002
H	-0.02051	4.27438	-1.56175	H	-2.34140	-3.33092	1.72114
H	-4.39143	3.50502	0.64439	H	-3.73760	0.72779	4.20314
H	-1.63351	6.14405	-1.28996	H	-4.04098	-3.48731	3.52632
O	0.80433	1.79791	-1.23009	O	-0.62985	-2.05533	0.19443
N	-0.73883	0.50689	-0.36899	N	-0.55021	0.09495	0.62464
O	2.81020	1.41920	0.70207	O	-0.23083	-4.54584	-3.09458
C	2.83500	2.82664	0.91690	C	-0.83590	-5.44709	-4.01769
H	2.60443	3.28375	-0.04572	H	-0.18366	-6.32292	-4.06027
H	3.85190	3.13437	1.19582	H	-0.85389	-5.00732	-5.02271
H	2.87433	0.92975	1.56279	H	-0.67025	-3.67581	-3.17326
H	-3.81549	5.72377	-0.18414	H	-4.71341	-1.43783	4.75370
C	1.84757	3.29941	1.97352	C	-2.24110	-5.86218	-3.60616
H	1.89438	4.38704	2.07502	H	-2.65390	-6.58228	-4.31828
H	0.82759	3.02307	1.70320	H	-2.23195	-6.32308	-2.61624
H	2.07472	2.85922	2.94706	H	-2.90698	-4.99672	-3.57422
C	-2.83833	1.24477	0.50170	C	-1.86638	1.23669	2.26067
C	-1.93098	0.24183	0.25395	C	-0.93608	1.24878	1.24759
C	-4.11076	1.01719	1.27532	C	-2.27677	2.48414	2.99832
H	-4.21157	1.76465	2.06607	H	-3.35209	2.66089	2.90480
H	-4.99859	1.09524	0.64040	H	-2.05670	2.39877	4.06639
H	-4.12602	0.04189	1.74944	H	-1.77001	3.36410	2.61821
C	-2.07416	-1.21672	0.67744	C	-0.26372	2.50108	0.69903
O	-1.73905	-1.36949	2.05029	O	-1.20795	3.47042	0.23885
C	-3.39665	-1.89569	0.36664	C	0.71069	3.17459	1.65342
C	-4.01772	-1.70284	-0.86965	C	1.50187	2.40949	2.51304
C	-3.96841	-2.79075	1.26967	C	0.88431	4.55877	1.63574
C	-5.18555	-2.38306	-1.19315	C	2.44307	3.01414	3.33855
C	-5.14093	-3.46939	0.94814	C	1.82241	5.16414	2.46669
C	-5.75427	-3.26963	-0.28312	C	2.60624	4.39567	3.31986
H	-3.59406	-1.00466	-1.58268	H	1.37738	1.33360	2.54710
H	-3.49184	-2.94716	2.22757	H	0.27653	5.16110	0.97474
H	-5.65464	-2.21685	-2.15610	H	3.04530	2.40427	4.00199
H	-5.57472	-4.15753	1.66477	H	1.93965	6.24156	2.44521
H	-6.66695	-3.79787	-0.53253	H	3.33587	4.86832	3.96673
H	-0.79477	-1.08460	2.10984	H	-1.78003	3.04193	-0.42001
H	-1.32387	-1.74707	0.08207	H	0.31910	2.15227	-0.16023
TS24				INT24			
Ru	1.08702	-0.84439	-0.39230	Ru	1.40763	-0.40446	-0.28150
C	1.37138	-3.02869	-0.66032	C	2.40787	-2.34495	-0.68103
C	0.08684	-2.66432	-1.15835	C	1.07964	-2.42810	-1.20150
C	0.03264	-1.61729	-2.12321	C	0.66917	-1.40746	-2.08832
C	1.20077	-0.97943	-2.60063	C	1.55040	-0.37306	-2.50608

C	2.46060	-1.32860	-2.06913	C	2.85602	-0.30683	-1.99327
C	2.52915	-2.37282	-1.09552	C	3.27031	-1.30979	-1.05721
H	1.45707	-3.73547	0.14833	H	2.73311	-3.02868	0.08636
H	-0.93421	-1.26977	-2.46466	H	-0.35659	-1.39327	-2.43362
H	1.11801	-0.14295	-3.27965	H	1.18367	0.42052	-3.13934
H	3.47115	-2.58764	-0.61190	H	4.23594	-1.22832	-0.57799
C	-1.17451	-3.41242	-0.77993	C	0.15424	-3.58871	-0.89594
C	-1.22533	-3.88860	0.67351	C	0.28957	-4.16155	0.51682
C	-1.34403	-4.59520	-1.75338	C	0.38066	-4.68409	-1.95573
H	-2.01384	-2.73117	-0.94475	H	-0.86889	-3.22217	-1.01711
H	-1.09777	-3.06406	1.37437	H	0.14466	-3.39503	1.27703
H	-2.19334	-4.35286	0.86872	H	-0.46321	-4.93705	0.66732
H	-0.45722	-4.63552	0.88323	H	1.26666	-4.62295	0.67544
H	-1.36123	-4.26283	-2.79301	H	0.22866	-4.30315	-2.96725
H	-0.52856	-5.31361	-1.63970	H	1.39567	-5.08429	-1.89261
H	-2.28222	-5.11370	-1.54750	H	-0.31702	-5.50805	-1.79451
C	3.69772	-0.59845	-2.48834	C	3.79278	0.79092	-2.39238
H	4.44030	-0.60176	-1.69271	H	4.46822	1.05112	-1.57804
H	4.12971	-1.09994	-3.36007	H	4.40514	0.45064	-3.23301
H	3.46982	0.43089	-2.75852	H	3.24806	1.68019	-2.70251
O	0.79646	-0.85260	1.69939	O	0.98166	-0.85884	1.76398
C	1.35785	-1.68309	2.54155	C	1.87482	-1.36450	2.56902
O	1.98356	-2.69460	2.25109	O	2.97529	-1.79879	2.24463
C	1.15197	-1.28019	3.99355	C	1.42611	-1.38666	4.02311
H	1.73146	-1.92747	4.64786	H	2.21565	-1.78955	4.65317
H	1.44314	-0.23991	4.14367	H	1.17192	-0.37760	4.35244
H	0.09478	-1.36614	4.25761	H	0.53053	-2.00259	4.13352
C	0.88203	4.42183	-1.00513	C	-0.91464	4.49424	-1.07453
C	0.11923	3.33724	-0.53546	C	-1.13075	3.21592	-0.52563
C	-1.16587	3.54650	0.02039	C	-2.28910	2.95543	0.23992
C	-1.64496	4.87719	0.08365	C	-3.20644	4.01490	0.43902
C	-0.88670	5.92620	-0.38518	C	-2.97655	5.25898	-0.10292
C	0.38723	5.70383	-0.93511	C	-1.82388	5.50594	-0.86781
C	0.63984	1.99194	-0.59668	C	-0.14789	2.16946	-0.71347
H	1.85994	4.22358	-1.42410	H	-0.01922	4.65916	-1.65810
H	-2.62323	5.07662	0.49903	H	-4.10448	3.84702	1.01740
H	0.97299	6.53837	-1.30098	H	-1.65450	6.48880	-1.29084
O	1.82095	1.72182	-1.01054	O	0.92124	2.40923	-1.38368
N	-0.13396	0.96776	-0.21368	N	-0.35644	0.95333	-0.17334
H	-1.27790	6.93571	-0.32991	H	-3.69357	6.05554	0.06013
C	-1.92346	2.42038	0.48935	C	-2.50253	1.62890	0.73651
C	-1.39053	1.16704	0.31593	C	-1.55955	0.67173	0.45879
C	-3.24263	2.66040	1.17622	C	-3.75321	1.33427	1.52356
H	-3.13466	3.42970	1.94479	H	-3.86727	2.05934	2.33366

H	-4.01093	3.00631	0.47798	H	-4.65042	1.40183	0.90116
H	-3.61528	1.76734	1.66538	H	-3.72621	0.35029	1.97730
C	-2.06384	-0.12181	0.76861	C	-1.77888	-0.79772	0.80334
O	-1.93986	-0.27747	2.18314	O	-1.70405	-1.03200	2.20758
C	-3.49868	-0.33937	0.32813	C	-3.04376	-1.41364	0.22488
C	-3.88749	-0.02802	-0.97703	C	-3.47285	-1.08070	-1.06219
C	-4.42770	-0.93606	1.17957	C	-3.74618	-2.39051	0.93040
C	-5.17734	-0.29841	-1.41792	C	-4.57946	-1.70388	-1.62759
C	-5.72139	-1.20256	0.73967	C	-4.85751	-3.01108	0.36702
C	-6.10202	-0.88573	-0.55916	C	-5.27916	-2.67182	-0.91353
H	-3.18030	0.44050	-1.65229	H	-2.94571	-0.31998	-1.62635
H	-4.13348	-1.18509	2.18987	H	-3.42037	-2.65630	1.92663
H	-5.46192	-0.04599	-2.43289	H	-4.89829	-1.42838	-2.62631
H	-6.43300	-1.66094	1.41690	H	-5.39493	-3.76306	0.93359
H	-7.10936	-1.09309	-0.90045	H	-6.14496	-3.15466	-1.35114
H	-0.98184	-0.39628	2.32095	H	-0.74957	-0.93769	2.39155
H	-1.47649	-0.91508	0.29903	H	-0.94637	-1.32538	0.33466
H	3.02909	2.00198	-0.13714	H	2.00052	2.81437	-0.64864
O	3.85590	2.10335	0.45733	O	2.80719	3.12440	-0.01057
O	3.45163	-0.06938	0.83900	O	2.54542	1.08361	0.89539
C	4.11639	0.93932	1.02580	C	3.05282	2.21342	0.87801
C	5.31875	0.97400	1.93084	C	4.02154	2.61931	1.95338
H	6.19218	1.31722	1.37360	H	3.55178	3.37687	2.58470
H	5.14733	1.68951	2.73744	H	4.29903	1.76175	2.56000
H	5.50548	-0.01237	2.34676	H	4.90610	3.07241	1.50434
TS25				TS21b			
Ru	-1.58170	-0.12513	-0.22764	Ru	-0.56121	-0.98840	0.41150
C	-2.67153	1.15641	-1.64324	C	-1.32756	-0.94538	2.59212
C	-1.35174	1.02760	-2.16636	C	-1.86239	0.21872	1.95583
C	-0.85484	-0.28493	-2.31230	C	-2.69897	0.00859	0.82208
C	-1.64792	-1.43286	-2.03370	C	-2.94003	-1.27957	0.31994
C	-2.95654	-1.29497	-1.53999	C	-2.44121	-2.43529	1.00229
C	-3.45552	0.02997	-1.32912	C	-1.67664	-2.24805	2.17359
H	-3.06219	2.12958	-1.39206	H	-0.66308	-0.83281	3.44291
H	0.17724	-0.42535	-2.60935	H	-3.11415	0.86637	0.30158
H	-1.20842	-2.41666	-2.10879	H	-3.53409	-1.40381	-0.58153
H	-4.41729	0.17376	-0.85818	H	-1.28174	-3.10783	2.70868
C	-0.51503	2.21739	-2.58976	C	-1.71530	1.61082	2.54716
C	-0.75943	3.48810	-1.77223	C	-0.40094	1.84709	3.30461
C	-0.74105	2.47846	-4.09060	C	-2.93726	1.89176	3.45410
H	0.53150	1.93005	-2.45848	H	-1.76091	2.31764	1.71276
H	-0.63033	3.31179	-0.70430	H	0.47125	1.59185	2.69677
H	-0.05006	4.25907	-2.07673	H	-0.32903	2.90372	3.58247
H	-1.76292	3.88786	-1.93480	H	-0.35785	1.26898	4.23495

H	-0.51170	1.59627	-4.69119	H	-3.88131	1.78805	2.90914
H	-1.77903	2.76004	-4.28524	H	-2.95985	1.20622	4.30888
H	-0.10127	3.29571	-4.42912	H	-2.88195	2.91409	3.84219
C	-3.78051	-2.48489	-1.16258	C	-2.80335	-3.81452	0.52138
H	-4.35274	-2.28427	-0.25743	H	-2.06875	-4.55905	0.83533
H	-4.48521	-2.71117	-1.96818	H	-3.77389	-4.09514	0.94975
H	-3.15166	-3.35676	-0.99235	H	-2.89924	-3.84923	-0.56563
O	-1.36773	1.41416	1.21807	O	3.48894	1.74294	-1.83517
C	-2.33641	2.21486	1.57217	C	4.43309	1.75656	-0.99296
O	-3.45042	2.25639	1.06181	O	4.31934	1.57501	0.26455
C	-1.96685	3.12926	2.72855	C	5.85455	1.98515	-1.51413
H	-2.75839	3.85474	2.90032	H	5.84387	2.44580	-2.50466
H	-1.82461	2.53339	3.63312	H	6.42543	2.60370	-0.81597
H	-1.02723	3.64593	2.52730	H	6.36427	1.01725	-1.58745
C	1.72635	-4.52951	-0.19496	C	0.99505	-3.91196	-0.67575
C	1.73843	-3.16903	0.13598	C	1.00252	-2.50078	-0.83942
C	2.95150	-2.47222	0.27615	C	0.15863	-1.88028	-1.81841
C	4.14686	-3.18909	0.07483	C	-0.66744	-2.74109	-2.60115
C	4.12394	-4.53074	-0.25899	C	-0.64686	-4.11353	-2.44153
C	2.91027	-5.21109	-0.39639	C	0.19406	-4.70821	-1.47106
C	0.46585	-2.48538	0.37780	C	2.00422	-1.67590	-0.04593
H	0.77093	-5.02956	-0.28270	H	1.65618	-4.35735	0.06415
H	5.10070	-2.68999	0.17035	H	-1.31027	-2.29687	-3.35734
H	2.90023	-6.26318	-0.65380	H	0.21521	-5.78960	-1.35827
O	-0.60104	-3.09202	0.42241	O	3.19495	-1.58964	-0.32021
N	0.49396	-1.09331	0.59965	N	1.28557	-1.16688	1.01366
H	5.05835	-5.05760	-0.41479	O	2.40557	0.52289	1.62160
C	2.93474	-1.05082	0.58705	C	3.12269	0.08309	2.78633
C	1.74367	-0.40095	0.63486	H	3.93264	-0.59245	2.48579
C	4.26185	-0.39553	0.87514	H	2.41114	-0.48850	3.38885
H	4.81942	-1.01353	1.58288	H	3.09904	0.88766	0.94810
H	4.88060	-0.28846	-0.02015	H	-1.27609	-4.74109	-3.06880
H	4.15153	0.58513	1.32115	C	3.67436	1.26787	3.57972
C	1.54228	1.10384	0.77439	H	4.19434	0.90264	4.47379
O	1.21392	1.43035	2.12319	H	4.38267	1.84222	2.97610
C	2.61183	2.03231	0.21987	H	2.86662	1.93393	3.89946
C	3.06593	1.88087	-1.09292	C	0.24056	-0.41658	-2.14885
C	3.08405	3.10825	0.96842	C	-0.07058	0.35850	-1.09669
C	3.98098	2.77215	-1.63793	C	0.61483	-0.03382	-3.56422
C	4.00499	4.00064	0.42482	H	1.61496	-0.41397	-3.80743
C	4.45799	3.83736	-0.87849	H	-0.08324	-0.47853	-4.28454
H	2.71448	1.04753	-1.69112	H	0.61331	1.04741	-3.69066
H	2.72778	3.23972	1.98067	C	-0.02429	1.87223	-0.96097
H	4.32350	2.63470	-2.65713	O	0.91484	2.47982	-1.84790

H	4.36573	4.82831	1.02482	C	-1.36112	2.57051	-1.21585
H	5.17344	4.53265	-1.30141	C	-2.31421	2.07239	-2.11583
H	0.23813	1.45916	2.13560	C	-1.61521	3.79694	-0.58078
H	0.65631	1.30585	0.16533	C	-3.49770	2.77710	-2.36864
H	-0.10620	-0.97656	1.64184	C	-2.79575	4.50522	-0.82873
O	-0.76516	-1.12507	2.76933	C	-3.74426	3.99482	-1.72394
O	-2.55988	-1.01220	1.43702	H	-2.13521	1.12611	-2.61953
C	-1.99954	-1.27229	2.53938	H	-0.87579	4.20592	0.10627
C	-2.86349	-1.81793	3.64752	H	-4.22697	2.37480	-3.06897
H	-2.68638	-2.89336	3.72485	H	-2.97460	5.45313	-0.32545
H	-2.57862	-1.36698	4.59766	H	-4.66482	4.54123	-1.91769
H	-3.91776	-1.64614	3.44453	H	1.83029	2.11146	-1.69111
				H	0.27144	2.08894	0.07639

**Frequencies of some stationary points for the overall catalytic cycle,
computed at B3LYP+IDSCRF/TZP-DKH(-dfg) level in DCE**

Species	Frequencies (cm ⁻¹)
1a	43 59 84 105 130 211 252 279 324 383 409 415 482 521 563 634 686 709 722 805 813 855 864 909 953 1000 1002 1018 1021 1045 1058 1104 1107 1163 1183 1194 1201 1277 1323 1332 1356 1392 1413 1475 1481 1486 1491 1504 1529 1620 1641 1713 3027 3039 3087 3102 3120 3163 3172 3179 3187 3195 3471
2a	20 23 67 128 146 234 267 304 336 365 415 421 510 582 635 646 714 776 797 854 859 938 981 992 1010 1022 1051 1053 1055 1101 1149 1180 1200 1213 1245 1301 1347 1374 1403 1415 1474 1475 1489 1530 1626 1643 2338 3029 3043 3087 3087 3155 3161 3170 3177 3185 3619
3a	20 25 34 75 94 140 148 178 212 239 262 279 296 313 355 412 424 430 443 470 488 527 548 567 598 628 633 639 702 709 722 740 768 778 800 819 845 861 901 906 939 963 979 985 1005 1015 1018 1022 1024 1041 1050 1087 1109 1122 1133 1159 1176 1183 1183 1200 1205 1247 1265 1311 1330 1333 1348 1361 1370 1412 1421 1477 1483 1490 1496 1502 1506 1528 1617 1631 1635 1652 1703 1723 3040 3043 3106 3132 3140 3165 3165 3175 3175 3182 3184 3189 3198 3200 3529
4a	19 36 38 94 126 147 185 195 220 236 240 264 299 305 360 368 388 414 439 466 501 516 536 567 609 628 635 649 686 710 714 724 752 785 798 816 818 849 857 897 900 940 990 992 1011 1014 1022 1048 1054 1061 1068 1089 1100 1108 1150 1178 1181 1189 1202 1205 1212 1264 1290 1306 1313 1351 1357 1365 1385 1419 1444 1460 1491 1494 1496 1507 1523 1531 1590 1626 1641 1645 1660 1680 2975 3023 3061 3153 3163 3165 3173 3180 3184 3186 3196 3199 3208 3485 3625
HOAc	63 432 544 588 651 868 1003 1069 1198 1345 1410 1467 1473 1769 3053 3110 3161 3507
EtOH	259 293 423 807 882 1055 1069 1130 1285 1379 1403 1415 1485 1489 1515 2996 3023 3065 3087 3099 3667
LRu(OAc) ₂	26 28 35 45 59 65 71 89 110 128 152 174 189 195 204 227 235 243 259 272 287 299 328 353 384 400 416 450 456 491 519 529 571 623 627 647 669 676 690 697 814 892 904 920 932 940 962 966 971 979 1007 1018 1021 1031 1060 1061 1069 1079 1109 1135 1166 1180 1221 1235 1309 1335 1336 1361 1384 1388 1401 1415 1418 1424 1427 1449 1466 1466 1473 1477 1487 1491 1492 1495 1499 1502 1510 1532 1537 1569 1645 3025 3029 3033 3035 3045 3050 3091 3096 3096 3100 3103 3107 3112 3132 3137 3145 3178 3191 3208 3219

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	71	74	79	81	102	105	115	128	135	143	175	186
	199	204	216	224	237	240	249	260	268	278	287	297
	313	328	355	391	392	401	416	434	439	441	447	485
	520	523	528	540	579	626	629	634	645	662	671	674
	689	693	696	712	730	804	814	816	855	867	893	910
	915	921	935	942	953	966	971	983	992	1000	1002	1008
	1018	1019	1021	1023	1032	1047	1054	1062	1063	1071	1082	1103
	1108	1136	1166	1169	1182	1182	1194	1199	1223	1238	1292	1309
	1330	1331	1346	1356	1361	1385	1388	1389	1402	1412	1417	1418
	1426	1449	1465	1473	1473	1476	1480	1482	1486	1487	1488	1489
	1503	1503	1506	1512	1520	1522	1533	1543	1566	1619	1641	1647
	1700	3025	3032	3035	3037	3043	3046	3047	3053	3088	3088	3094
	3097	3100	3103	3107	3113	3115	3129	3139	3149	3162	3171	3174
	3180	3187	3192	3195	3213	3229	3411					
TS1	-53	9	25	27	34	42	44	48	49	49	53	55
	68	70	75	75	97	97	105	113	131	149	157	165
	177	184	202	205	221	235	239	241	264	281	284	299
	316	334	353	358	382	395	413	415	427	447	450	489
	518	530	53									
INT1	12	29	35	35	43	48	49	54	60	65	73	81
	87	89	91	103	106	120	135	148	158	169	178	187
	187	198	208	219	222	239	241	253	268	276	286	304
	318	347	356	368	394	410	417	418	430	438	446	513
	514	524	528	549	580	621	627	634	641	675	675	679
	685	693	708	741	818	820	830	849	868	878	894	908
	922	929	935	941	961	969	971	991	999	1008	1008	1021
	1023	1028	1031	1033	1035	1049	1054	1062	1063	1066	1080	1108
	1109	1122	1135	1145	1169	1175	1184	1185	1211	1222	1239	1250
	1299	1311	1335	1336	1339	1359	1369	1370	1388	1400	1402	1409
	1410	1413	1418	1419	1425	1462	1466	1471	1476	1477	1481	1483
	1486	1488	1493	1498	1503	1510	1515	1516	1522	1527	1554	1564
	1590	1620	1639	1641	1731	2870	3018	3024	3029	3035	3037	3042
	3045	3046	3058	3087	3093	3097	3103	3104	3108	3109	3113	3115
	3135	3137	3141	3165	3176	3181	3185	3195	3202	3213	3222	3230
TS2	-713	19	20	38	40	43	45	47	51	62	65	68
	74	81	85	93	111	113	125	138	151	165	176	181
	192	199	202	216	223	237	242	258	267	271	279	297
	311	327	349	363	379	395	401	418	423	436	444	449
	520	525	533	549	581	604	622	634	639	643	674	679
	693	694	712	723	750	817	827	832	864	867	893	908
	921	923	936	940	941	956	971	985	989	995	1003	1009
	1016	1022	1026	1032	1041	1045	1051	1054	1061	1069	1081	1095
	1108	1114	1136	1147	1167	1173	1182	1183	1205	1221	1237	1268
	1296	1310										

	1328 1336 1338 1359 1359 1384 1386 1395 1401 1401 1414 1416 1417 1417 1424 1444 1460 1465 1472 1476 1478 1480 1480 1486 1488 1493 1498 1504 1505 1512 1516 1528 1529 1567 1584 1619 1638 1641 1654 1678 3011 3025 3031 3036 3038 3039 3044 3048 3050 3087 3093 3097 3102 3104 3104 3109 3111 3114 3134 3137 3155 3162 3171 3181 3182 3188 3202 3224 3226 3234
INT2	26 33 37 39 47 51 55 60 62 67 71 76 80 81 102 105 119 131 139 151 160 174 180 189 200 205 211 215 223 235 242 245 259 272 278 297 310 352 362 369 386 412 415 415 418 449 455 485 510 513 516 568 588 615 618 635 642 649 667 694 695 698 714 743 800 818 828 866 867 892 907 922 928 930 939 943 945 972 977 984 989 998 1005 1009 1021 1026 1032 1038 1045 1051 1059 1060 1063 1072 1080 1100 1106 1140 1144 1159 1163 1177 1179 1187 1199 1220 1237 1288 1301 1314 1320 1328 1344 1358 1358 1370 1390 1394 1400 1413 1413 1415 1420 1426 1428 1458 1467 1474 1477 1477 1478 1481 1486 1489 1493 1498 1500 1505 1510 1516 1529 1538 1546 1575 1588 1619 1640 1675 1688 2526 3012 3029 3033 3035 3037 3040 3045 3051 3055 3092 3095 3098 3101 3102 3103 3106 3112 3118 3126 3146 3158 3160 3166 3176 3184 3188 3202 3208 3231 3252
INT3	15 21 29 38 39 51 54 59 61 65 67 72 77 80 91 98 106 109 118 124 127 137 142 169 186 192 199 214 221 222 239 249 262 265 282 297 313 345 347 354 366 392 403 427 439 447 451 453 504 510 519 568 575 604 616 623 634 637 671 680 697 705 708 749 804 818 824 867 887 893 895 918 931 931 940 944 952 960 973 980 994 1001 1015 1017 1019 1020 1024 1031 1034 1041 1049 1059 1066 1069 1083 1104 1117 1139 1141 1163 1168 1172 1179 1191 1195 1219 1239 1268 1286 1302 1317 1329 1334 1342 1356 1360 1382 1392 1397 1402 1414 1415 1419 1421 1427 1430 1465 1468 1474 1475 1477 1479 1481 1486 1491 1493 1497 1502 1507 1514 1516 1517 1550 1572 1611 1629 1642 1654 1735 2883 3016 3027 3029 3035 3037 3039 3051 3051 3071 3090 3096 3100 3102 3104 3108 3110 3110 3111 3129 3147 3156 3165 3175 3185 3185 3187 3190 3198 3211 3212
TS3	-1195 22 34 44 49 51 56 62 66 77 92 97 127 137 144 153 179 181 192 205 209 226 235 241 249 258 270 280 300 307 328 337 351 353 373 388 406 442 447 447 480 512 521 550 565 569 635 640 660 671 685 695 707 722 769 811 813 825 866 889 895 905 918 932 940 949 971 972 983 989 1003 1012 1017 1019 1032 1040 1043 1057 1060 1069 1081 1106 1113 1136 1141 1161 1174 1176 1178 1185 1199 1220 1236 1283 1287 1313 1326 1334

	1338 1358 1361 1389 1392 1401 1412 1414 1420 1422 1425 1455 1471 1473 1475 1481 1483 1487 1488 1493 1496 1498 1498 1504 1512 1519 1545 1575 1595 1611 1618 1642 3025 3027 3029 3034 3035 3035 3052 3064 3091 3096 3096 3099 3100 3105 3105 3111 3125 3150 3152 3162 3174 3179 3183 3187 3195 3213
INT4	13 19 28 32 41 44 46 58 69 78 88 92 97 106 123 128 142 164 171 185 197 220 228 232 243 256 259 273 295 323 345 358 380 383 393 426 432 440 449 451 497 513 527 569 590 603 618 647 666 678 689 715 728 763 801 820 823 865 877 885 890 903 906 928 939 965 970 975 980 981 1000 1003 1009 1013 1022 1040 1043 1054 1064 1068 1075 1108 1120 1136 1142 1159 1168 1175 1176 1180 1227 1233 1261 1276 1286 1294 1304 1335 1337 1355 1387 1393 1401 1410 1416 1419 1424 1441 1441 1469 1472 1474 1475 1475 1482 1486 1487 1490 1495 1499 1502 1510 1515 1518 1575 1601 1612 1629 1744 3010 3023 3028 3029 3036 3039 3044 3050 3090 3092 3095 3099 3102 3107 3110 3115 3117 3123 3141 3154 3158 3167 3178 3182 3189 3191 3209
TS4	-28 12 17 22 25 26 29 32 35 38 48 51 53 58 65 70 74 82 86 90 101 106 114 132 138 145 150 170 177 182 185 201 208 229 229 242 257 260 280 288 288 311 326 328 343 371 378 385 387 394 41
INT5	16 28 32 33 37 44 47 55 58 60 69 71 77 80 92 104 108 115 117 119 130 131 138 150 163 167 172 181 190 199 210 215 220 238 245 254 257 271 278 286 291 316 327 340 348 357 369 379 384 394 411 415 435 444 450 462 466 516 521 534 550 571 578 582 609 614 634 635 641 666 667 682 699 713 718 722 753 768 804 816 820 821 844 859 870 887 894 901 902 926 933 934 940 969 971 977 991 991 1003 1006 1009 1013 1021 1024 1032 1033 1038 1039 1043 1050 1058 1059 1066 1069 1082 1100 1101 1105 1107 1120 1135 1141 1160 1173 1176 1179 1188 1194 1197 1208 1219 1238 1269 1284 1285 1310 1321 1321 1325 1334 1346 1360 1371 1378 1388 1391 1396 1401 1407 1413 1415 1418 1425 1455 1457 1470 1470 1472 1475 1476 1478 1480 1482 1487 1488 1489 1493 1498 1504 1509 1516 1520 1529 1559 1575 1581 1601 1619 1626 1641 1700 2081 2643 3014 3025 3027 3030 3033 3036 3040 3051 3060 3070 3085 3089 3095 3099 3099 3103 3105 3106 3107 3116 3129 3142 3155 3155 3159 3162 3168 3170 3176 3179 3181 3182 3185 3191 3212 3525
TS5	-294 21 28 31 36 43 47 48 54 58 65 70 74 75 85 90 104 107 111 114 124 133 145 161 173 178 180 190 196 197 206 222 234 245 251 258

	269	270	277	293	309	318	338	344	350	358	370	379
	390	407	414	417	440	444	453	460	476	500	519	523
	530	569	575	588	607	625	632	638	639	654	681	695
	703	714	716	740	765	779	808	818	819	824	860	865
	870	884	894	895	899	917	931	936	942	960	970	975
	976	992	1003	1005	1006	1008	1011	1015	1022	1030	1030	1039
	1042	1051	1057	1060	1061	1069	1072	1076	1093	1105	1111	1120
	1134	1142	1163	1174	1178	1179	1182	1188	1199	1205	1217	1236
	1257	1266	1285	1311	1314	1327	1327	1338	1347	1358	1369	1376
	1393	1396	1398	1399	1402	1413	1416	1419	1425	1427	1460	1463
	1473	1475	1476	1478	1480	1482	1482	1486	1488	1489	1493	1500
	1503	1504	1515	1519	1531	1553	1572	1575	1595	1615	1626	1643
	1709	1855	2709	3014	3015	3026	3031	3032	3034	3038	3050	3056
	3059	3089	3089	3092	3097	3098	3102	3107	3108	3109	3111	3121
	3151	3154	3156	3162	3165	3171	3173	3178	3182	3185	3187	3190
	3192	3213	3621									
INT6	22	25	30	34	43	49	50	55	64	65	68	73
	77	80	89	90	100	101	114	123	129	135	139	148
	150	164	170	179	189	200	210	228	240	246	248	257
	269	273	276	294	302	321	338	347	351	368	374	383
	397	403	418	434	443	456	460	509	525	528	539	552
	557	569	583	605	607	623	636	642	659	680	684	690
	717	736	749	769	773	781	808	818	823	849	851	863
	866	884	889	894	895	913	931	940	943	971	978	981
	983	994	1003	1006	1009	1012	1013	1019	1022	1028	1031	1041
	1045	1051	1054	1056	1069	1073	1081	1091	1108	1110	1136	1137
	1142	1168	1175	1179	1181	1183	1188	1191	1199	1220	1236	1251
	1260	1286	1286	1296	1308	1314	1326	1342	1349	1356	1371	1385
	1391	1399	1401	1403	1407	1410	1416	1418	1421	1428	1453	1467
	1470	1474	1475	1476	1482	1486	1487	1489	1490	1492	1497	1498
	1502	1504	1516	1520	1529	1529	1574	1576	1624	1629	1636	1642
	1686	1724	2883	3002	3010	3013	3025	3030	3033	3040	3047	3048
	3049	3050	3086	3093	3097	3100	3104	3107	3112	3113	3134	3153
	3154	3154	3160	3160	3168	3170	3176	3180	3184	3185	3189	3190
	3200	3207	3659									
TS6	-640	21	23	36	38	39	40	47	51	54	60	61
	64	80	84	94	97	105	108	122	136	139	155	162
	162	168	179	183	190	208	213	217	229	238	241	250
	260	265	280	283	297	309	314	341	357	366	384	392
	400	407	414	416	444	450	461	476	506	526	530	569
	571	586	594	608	625	626	636	637	655	679	686	689
	694	710	714	748	768	783	791	799	806	817	825	861
	864	875	883	890	895	899	913	925	940	948	953	963
	970	971	982	988	998	999	1003	1011	1021	1030	1031	1043
	1044	1047	1049	1059	1060	1069	1071	1077	1085	1100	1107	1132
	1133	1143	1161	1170	1174	1180	1182	1183	1192	1207	1217	1231
	1238	1276										

	1287 1305 1313 1314 1317 1330 1336 1354 1360 1382 1389 1395 1397 1398 1401 1407 1414 1415 1421 1424 1463 1473 1475 1480 1480 1481 1483 1485 1486 1487 1488 1492 1499 1502 1504 1511 1512 1517 1530 1550 1555 1572 1603 1622 1635 1641 1707 1742 1961 2701 3016 3020 3024 3028 3030 3035 3037 3050 3051 3065 3089 3094 3097 3097 3101 3107 3108 3109 3115 3133 3154 3158 3159 3166 3168 3175 3178 3181 3182 3184 3185 3190 3192 3211 3528
INT7	23 28 36 38 42 44 48 55 59 62 66 66 82 89 95 99 103 108 119 129 132 139 144 157 170 174 180 189 198 208 222 226 231 240 249 253 259 268 270 278 299 318 331 352 357 382 394 403 405 415 418 443 444 451 463 497 527 530 569 572 577 587 594 608 627 632 635 644 672 677 683 689 699 711 718 748 762 777 788 791 801 818 819 827 861 866 877 890 896 899 911 926 941 944 957 963 971 971 984 988 998 999 1002 1009 1019 1031 1035 1039 1044 1045 1047 1060 1061 1069 1073 1076 1084 1101 1108 1132 1135 1144 1163 1171 1175 1179 1184 1184 1193 1217 1220 1238 1250 1279 1287 1311 1312 1313 1318 1333 1336 1355 1361 1385 1386 1394 1400 1402 1406 1414 1415 1415 1420 1424 1463 1473 1475 1479 1480 1481 1483 1484 1485 1488 1492 1492 1499 1502 1507 1513 1515 1519 1529 1551 1553 1581 1605 1619 1635 1639 1709 1780 2116 2730 3013 3022 3027 3030 3030 3037 3037 3047 3050 3067 3090 3094 3096 3099 3101 3107 3109 3112 3115 3132 3154 3159 3159 3167 3168 3176 3178 3182 3185 3185 3188 3196 3200 3210 3541
TS7	-542 19 23 29 31 34 38 43 53 57 60 62 66 75 82 97 98 106 111 119 132 139 146 152 167 175 190 194 205 215 223 233 242 255 256 265 271 278 287 306 310 322 341 346 361 378 389 405 410 413 419 440 443 446 451 463 464 496 526 531 558 573 585 592 602 610 625 635 639 671 675 684 690 694 709 728 739 761 775 792 806 815 821 825 858 869 877 894 896 899 909 929 940 943 957 959 972 976 982 984 994 1000 1002 1006 1020 1031 1032 1043 1045 1048 1059 1062 1069 1073 1077 1083 1093 1105 1107 1133 1136 1143 1163 1172 1178 1179 1186 1191 1197 1217 1220 1237 1237 1284 1287 1303 1314 1315 1328 1331 1334 1355 1360 1372 1378 1393 1395 1397 1403 1405 1414 1415 1420 1427 1462 1475 1475 1479 1480 1480 1481 1484 1488 1492 1495 1497 1499 1502 1506 1513 1514 1517 1529 1551 1555 1578 1612 1617 1634 1640 1709 1740 2116 2674 3000 3020 3027 3030 3032 3037 3039 3050 3054 3074 3089 3091 3095 3099 3103 3107 3108 3115 3123 3123 3154 3158 3162 3167 3177 3179 3181 3185 3189 3192 3193 3198 3217 3220 3585

INT8	15	16	21	28	32	38	43	49	57	59	64	68
	70	71	79	83	96	105	116	131	138	149	158	172
	178	183	204	213	214	223	236	243	248	255	261	274
	299	305	315	318	333	341	359	370	373	391	396	405
	413	420	433	442	443	447	455	472	516	521	532	544
	558	573	576	578	592	597	633	637	645	651	669	672
	692	697	709	729	771	776	789	807	812	823	838	860
	863	876	878	892	897	903	917	934	941	949	955	971
	978	980	982	998	1000	1001	1002	1010	1013	1019	1024	1040
	1052	1058	1060	1069	1070	1082	1094	1105	1111	1123	1137	1142
	1161	1168	1172	1181	1186	1189	1202	1206	1219	1220	1237	1250
	1261	1284	1306	1318	1319	1329	1336	1343	1353	1358	1362	1365
	1390	1397	1400	1409	1412	1412	1415	1416	1421	1424	1466	1472
	1473	1479	1480	1482	1485	1489	1492	1497	1498	1503	1505	1510
	1513	1514	1519	1527	1549	1553	1574	1580	1611	1616	1636	1638
	1748	3008	3020	3020	3025	3028	3032	3035	3054	3065	3082	3086
	3088	3092	3096	3099	3104	3111	3113	3119	3158	3160	3164	3165
	3170	3175	3182	3185	3191	3198	3200	3208	3210	3218	3220	3224
	3501	3548										
TS8	-1339	20	26	28	34	36	47	50	55	58	66	67
	71	86	98	108	111	119	131	142	143	160	164	177
	184	191	203	215	224	226	240	246	249	258	269	276
	301	305	312	322	324	345	347	366	374	390	403	407
	411	417	428	441	445	453	466	488	497	515	531	557
	564	587	594	622	625	634	640	669	672	673	692	697
	706	723	729	767	780	806	812	817	823	852	862	866
	877	891	895	900	905	928	933	940	959	963	966	971
	978	982	983	1001	1003	1006	1018	1022	1023	1042	1046	1052
	1057	1064	1072	1080	1083	1100	1103	1109	1118	1122	1137	1141
	1160	1162	1171	1177	1181	1185	1191	1198	1207	1220	1233	1238
	1268	1284	1288	1319	1324	1328	1333	1343	1356	1357	1384	1391
	1393	1400	1406	1409	1413	1416	1418	1421	1425	1437	1448	1458
	1474	1476	1479	1481	1485	1486	1489	1493	1498	1499	1503	1507
	1507	1507	1514	1515	1525	1528	1547	1577	1582	1592	1613	1619
	1633	1636	1637	1943	3008	3017	3023	3026	3028	3033	3035	3052
	3064	3083	3087	3089	3093	3097	3100	3104	3112	3116	3120	3159
	3161	3162	3165	3173	3176	3181	3183	3190	3198	3200	3200	3203
	3217	3223	3225									
INT9	8	14	18	24	29	36	37	39	51	53	55	63
	68	69	86	93	103	104	112	121	135	141	155	161
	167	179	187	192	210	226	233	242	248	257	263	269
	284	299	306	316	331	335	358	366	393	396	407	413
	420	431	437	439	441	445	447	482	489	517	521	545
	553	590	595	600	611	629	633	647	673	678	695	698
	703	737	757	769	785	803	810	824	831	859	866	869
	878	880	883	891	897	904	920	925	943	961	972	978

	979 986 991 999 1002 1003 1015 1018 1019 1020 1028 1037 1050 1055 1062 1069 1075 1082 1088 1100 1105 1113 1125 1139 1140 1151 1167 1172 1183 1184 1188 1203 1205 1226 1236 1248 1251 1257 1261 1289 1305 1312 1324 1333 1333 1350 1358 1366 1382 1395 1401 1408 1411 1416 1421 1426 1427 1435 1468 1472 1474 1474 1479 1481 1483 1485 1489 1492 1497 1498 1503 1509 1509 1514 1515 1517 1522 1527 1576 1601 1614 1622 1632 1638 1669 1753 2972 2992 3014 3028 3028 3031 3037 3038 3051 3064 3075 3090 3091 3096 3100 3103 3108 3108 3118 3122 3140 3157 3159 3164 3165 3176 3176 3182 3184 3185 3194 3200 3209 3216 3224 3226 3322
INT10	18 21 30 40 49 56 57 66 69 71 81 83 92 105 107 119 128 134 146 151 159 164 171 179 188 197 213 218 227 229 233 248 251 257 270 275 282 297 301 311 327 330 362 368 369 391 403 410 416 420 426 434 438 445 474 484 489 510 522 548 559 587 593 616 627 634 641 644 671 681 695 699 709 729 759 775 786 808 809 824 846 854 858 867 875 891 895 899 914 916 922 938 966 966 968 970 976 978 996 1003 1006 1007 1017 1020 1020 1021 1034 1042 1051 1059 1060 1069 1072 1077 1091 1103 1107 1120 1135 1139 1145 1166 1172 1179 1181 1184 1189 1201 1207 1222 1230 1236 1258 1286 1292 1310 1319 1329 1331 1343 1347 1353 1358 1394 1395 1398 1404 1408 1415 1416 1419 1421 1425 1443 1460 1473 1474 1480 1481 1484 1488 1489 1492 1493 1497 1501 1503 1505 1509 1511 1511 1522 1526 1530 1578 1593 1616 1618 1634 1636 1686 1717 2812 2933 2982 3025 3030 3030 3038 3039 3049 3055 3090 3090 3093 3095 3097 3106 3107 3112 3118 3118 3130 3153 3157 3161 3165 3166 3172 3174 3182 3185 3188 3190 3195 3200 3201 3210 3215
TS9	-259 18 27 30 42 47 49 53 56 59 72 82 83 99 104 105 117 118 124 134 149 155 160 166 169 186 196 206 217 232 238 242 249 259 264 267 273 280 288 298 301 317 326 335 351 365 384 399 413 417 418 423 426 432 446 472 486 492 522 534 547 561 576 590 627 634 636 640 674 677 684 693 695 710 712 757 767 784 798 810 822 848 855 862 866 876 891 896 897 909 916 940 942 963 970 972 974 983 1000 1003 1004 1016 1018 1020 1022 1022 1037 1050 1056 1056 1067 1067 1074 1081 1090 1107 1110 1117 1118 1129 1142 1167 1178 1179 1181 1187 1188 1202 1208 1221 1235 1237 1240 1253 1298 1301 1311 1324 1331 1339 1353 1355 1378 1384 1393 1401 1404 1408 1410 1415 1416 1420 1428 1454 1470 1473 1478 1479 1480 1481 1489 1489 1491 1492 1495 1497 1500 1507 1508 1511 1514 1527 1539 1548 1565 1591 1603 1618 1619 1635 1636 1715 2623 2950 2996 3026 3029 3036 3037 3038 3039 3051 3089 3089 3094 3098 3099 3101 3108 3109

	3129 3132 3132 3142 3151 3160 3160 3161 3171 3175 3181 3181 3188 3188 3194 3198 3199 3206 3206
INT11	1 20 27 31 32 44 45 50 51 57 64 66 69 75 88 92 105 106 113 117 127 133 143 151 156 159 169 176 185 200 214 221 232 238 252 256 259 267 281 298 303 311 320 333 362 376 385 403 405 412 421 425 428 430 445 467 495 523 534 537 560 566 584 589 612 617 630 634 640 676 686 690 695 704 705 744 757 774 776 808 809 816 838 862 869 881 885 895 897 903 915 920 938 942 963 970 978 985 1004 1007 1009 1011 1017 1020 1021 1034 1034 1050 1052 1057 1060 1063 1067 1072 1085 1104 1106 1111 1120 1130 1140 1142 1153 1179 1180 1185 1194 1201 1208 1223 1224 1233 1245 1264 1297 1302 1317 1327 1332 1334 1338 1352 1354 1379 1388 1390 1394 1402 1403 1409 1415 1422 1429 1442 1442 1467 1474 1477 1480 1482 1487 1488 1488 1491 1491 1493 1501 1504 1509 1514 1527 1529 1532 1556 1603 1604 1619 1619 1629 1637 1643 1721 2966 3001 3008 3024 3027 3038 3039 3046 3047 3054 3087 3087 3090 3097 3097 3099 3101 3108 3111 3128 3131 3145 3162 3162 3172 3174 3177 3179 3182 3187 3192 3197 3199 3201 3214 3218 3606
TS10	-85 9 25 30 36 45 48 50 57 60 71 75 80 81 93 99 108 117 126 128 134 136 158 162 167 176 184 191 192 207 213 231 239 246 263 266 277 281 290 293 304 315 327 348 356 369 386 410 414 420 423 430 433 444 448 477 499 508 522 531 541 558 571 588 611 625 635 641 673 678 685 694 699 711 712 715 762 769 785 808 811 815 840 848 870 887 894 900 900 906 913 925 942 942 965 971 987 995 1002 1006 1010 1012 1015 1020 1024 1026 1039 1045 1054 1061 1064 1065 1066 1081 1082 1108 1109 1112 1117 1134 1146 1157 1168 1175 1181 1185 1192 1207 1223 1226 1237 1243 1252 1269 1298 1311 1315 1337 1338 1340 1354 1361 1365 1383 1397 1398 1403 1407 1413 1416 1420 1424 1429 1456 1464 1469 1477 1479 1481 1485 1487 1490 1491 1492 1493 1493 1495 1502 1504 1513 1516 1519 1531 1532 1579 1588 1608 1614 1621 1632 1641 1716 2974 3007 3008 3024 3028 3037 3039 3052 3053 3055 3086 3093 3099 3099 3101 3108 3114 3117 3129 3142 3148 3165 3170 3178 3180 3182 3183 3188 3190 3194 3195 3199 3201 3204 3217 3230 3493
INT12	16 20 27 30 33 38 43 52 56 57 59 62 71 82 95 108 111 120 124 138 145 151 157 165 167 180 186 193 195 216 225 226 240 244 258 262 269 272 273 299 316 324 339 345 361 381 392 409 422 425 430 438 441 446 477 510 518 525 545 565 578 588 611 623 632 638 644 653 661 670 673 694

	699 709 713 768 771 778 809 814 818 821 853 858 884 894 894 914 920 931 938 941 945 962 969 970 984 996 1004 1005 1005 1011 1019 1025 1025 1033 1037 1038 1054 1059 1060 1063 1078 1081 1104 1109 1113 1119 1127 1136 1143 1167 1172 1174 1185 1187 1190 1205 1221 1221 1238 1252 1277 1302 1304 1316 1335 1337 1345 1355 1357 1359 1364 1391 1394 1394 1401 1405 1408 1409 1409 1415 1425 1437 1448 1467 1470 1479 1483 1487 1487 1488 1492 1493 1494 1500 1501 1503 1505 1507 1513 1515 1528 1528 1565 1608 1620 1630 1634 1639 1655 1657 2999 3015 3023 3026 3032 3036 3038 3043 3046 3051 3085 3088 3094 3095 3095 3101 3103 3106 3111 3118 3122 3137 3144 3154 3164 3166 3167 3175 3177 3183 3186 3196 3201 3205 3220 3238 3582
TS11	-92 12 23 29 30 39 45 49 52 58 61 62 66 74 80 85 86 95 100 104 106 107 111 113 118 127 132 146 148 161 166 169 176 180 186 207 213 225 240 244 255 263 266 272 279 282 290 311 319 326 349 355 387 404 412 421 429 437 439 450 460 461 466 482 521 524 546 568 575 579 595 601 617 631 633 642 648 654 670 680 701 704 706 714 734 762 774 775 815 817 821 825 848 869 896 897 900 901 913 924 933 938 939 943 965 969 972 976 985 1006 1006 1008 1010 1019 1023 1024 1026 1029 1039 1040 1052 1058 1061 1062 1065 1069 1084 1087 1106 1110 1112 1119 1130 1139 1164 1175 1177 1180 1181 1188 1203 1209 1221 1224 1241 1247 1295 1304 1310 1313 1317 1332 1338 1354 1362 1363 1364 1374 1392 1395 1400 1402 1403 1410 1411 1420 1423 1428 1441 1445 1457 1464 1473 1476 1478 1479 1481 1484 1485 1488 1491 1492 1494 1496 1499 1501 1502 1506 1510 1517 1527 1532 1547 1563 1581 1622 1622 1635 1640 1651 1713 1721 2808 2972 3024 3027 3029 3029 3038 3039 3044 3045 3050 3052 3087 3094 3095 3097 3099 3101 3103 3111 3112 3123 3128 3133 3147 3154 3162 3164 3170 3171 3175 3179 3184 3188 3191 3199 3204 3208 3226 3235 3467
INT13	16 16 22 25 28 34 36 47 52 53 55 59 63 71 73 84 92 94 104 108 111 118 123 127 142 152 152 160 162 166 168 178 185 190 205 212 222 233 240 252 255 273 275 279 280 300 308 321 328 337 345 356 367 390 405 411 425 426 443 446 454 461 483 490 511 518 545 573 573 573 594 612 618 633 639 641 648 652 666 673 696 703 704 722 760 772 773 774 808 814 819 825 836 862 885 894 895 915 917 921 930 936 937 940 964 970 971 972 980 989 1003 1005 1007 1016 1018 1021 1024 1036 1039 1048 1050 1057 1060 1062 1074 1080 1083 1092 1105 1107 1112 1124 1137 1143 1151 1161 1176 1180 1182 1183 1198 1201 1216 1220 1237 1243 1295

	1307 1311 1315 1331 1334 1355 1356 1358 1361 1362 1388 1394 1395 1399 1401 1406 1409 1413 1414 1417 1423 1426 1445 1458 1463 1470 1471 1475 1479 1481 1483 1486 1489 1490 1490 1493 1497 1499 1499 1504 1505 1512 1513 1513 1527 1548 1551 1569 1612 1620 1637 1637 1648 1670 1724 2237 2991 3023 3026 3028 3029 3031 3036 3036 3042 3044 3045 3085 3088 3091 3094 3095 3098 3098 3107 3107 3109 3110 3140 3141 3151 3156 3162 3167 3172 3177 3182 3186 3190 3192 3197 3199 3201 3213 3232 3442
TS12	-1017 13 18 24 31 38 41 45 49 56 60 67 74 79 80 88 102 111 118 130 138 146 150 162 165 180 186 193 201 214 215 229 236 240 245 253 261 269 273 279 296 308 334 346 356 365 388 395 412 418 430 438 443 445 466 488 519 533 537 548 564 570 587 616 622 623 634 635 642 658 674 681 692 700 702 719 739 753 773 780 810 818 832 850 861 893 899 905 906 924 934 940 941 945 967 969 975 982 989 1001 1005 1007 1014 1019 1022 1024 1025 1031 1039 1040 1050 1053 1060 1064 1066 1074 1103 1109 1110 1132 1133 1151 1164 1175 1176 1183 1189 1191 1203 1222 1238 1242 1252 1309 1312 1317 1331 1338 1341 1341 1348 1357 1362 1368 1382 1387 1404 1414 1417 1418 1422 1428 1442 1460 1466 1475 1475 1477 1479 1484 1488 1490 1492 1493 1497 1499 1501 1509 1510 1512 1528 1536 1573 1617 1619 1635 1636 1636 1647 1659 1698 1739 3027 3034 3037 3039 3045 3052 3055 3090 3096 3099 3100 3104 3112 3112 3117 3121 3133 3136 3139 3153 3162 3163 3164 3174 3174 3179 3183 3184 3188 3195 3198 3203 3210 3228
TS10b	-401 15 23 26 32 36 40 42 50 51 59 64 70 72 80 89 99 105 113 118 122 131 151 156 169 179 186 189 192 208 219 226 238 248 256 264 282 296 301 321 330 336 341 349 364 364 381 399 405 416 422 436 441 445 448 476 501 516 548 548 566 573 584 598 605 609 626 633 638 661 685 686 699 709 725 766 770 777 805 806 823 827 846 852 857 869 879 881 891 891 898 911 936 940 952 954 961 967 972 996 998 1005 1012 1013 1014 1015 1017 1027 1029 1048 1050 1055 1068 1074 1077 1099 1101 1114 1128 1130 1134 1150 1157 1171 1179 1181 1183 1201 1215 1224 1229 1235 1247 1260 1279 1292 1307 1307 1329 1339 1350 1356 1358 1372 1378 1385 1396 1397 1400 1409 1410 1419 1419 1422 1453 1464 1467 1474 1476 1480 1481 1484 1485 1486 1487 1492 1497 1502 1503 1507 1511 1513 1519 1521 1529 1559 1609 1616 1620 1633 1644 1761 2924 2987 3020 3023 3023 3029 3033 3036 3052 3058 3063 3082 3084 3091 3094 3096 3108 3108 3110 3114 3114 3158 3163 3164 3171 3173 3174 3174 3175 3183 3184 3185 3190 3195 3198 3207 3387

TS21	-152	20	27	29	35	38	40	45	50	57	62	67
	72	78	84	96	100	107	113	123	129	146	154	157
	161	178	196	208	209	217	228	242	244	248	249	267
	269	276	293	299	308	321	341	365	377	386	391	402
	415	424	437	443	445	462	465	488	520	523	532	559
	567	586	591	601	609	632	635	636	660	676	678	691
	713	719	731	764	769	797	814	822	824	832	859	867
	867	884	892	898	902	908	930	936	938	942	968	970
	973	983	992	994	1000	1006	1021	1027	1028	1031	1032	1038
	1052	1060	1063	1070	1070	1077	1098	1104	1111	1130	1132	1141
	1173	1174	1179	1180	1185	1189	1200	1217	1234	1238	1262	1281
	1304	1313	1313	1332	1337	1339	1345	1358	1361	1384	1392	1393
	1400	1411	1414	1416	1420	1424	1456	1458	1470	1475	1480	1481
	1485	1485	1488	1492	1492	1497	1500	1502	1505	1513	1514	1519
	1551	1564	1566	1607	1625	1634	1639	1707	2857	3017	3024	3027
	3031	3033	3041	3046	3051	3065	3068	3086	3088	3094	3096	3103
	3108	3116	3116	3120	3156	3159	3159	3168	3174	3175	3178	3179
	3188	3194	3200	3206	3209	3524						
INT21	9	16	28	33	40	42	44	49	54	56	62	72
	77	80	84	94	100	112	119	130	132	144	159	177
	192	196	210	216	224	233	239	245	247	249	264	274
	277	290	307	317	323	346	351	387	399	404	415	418
	422	434	442	443	451	457	473	492	524	530	546	555
	562	573	601	609	612	630	636	642	673	682	688	701
	715	721	746	770	783	803	815	822	833	851	858	859
	868	885	887	889	892	901	907	934	937	939	952	955
	968	978	990	998	1000	1003	1015	1021	1024	1024	1025	1040
	1053	1058	1063	1070	1073	1077	1093	1102	1103	1114	1127	1144
	1162	1175	1178	1180	1188	1196	1217	1218	1233	1239	1259	1269
	1285	1299	1310	1325	1339	1342	1345	1357	1360	1379	1381	1394
	1399	1411	1418	1418	1419	1422	1428	1436	1467	1474	1482	1483
	1485	1485	1488	1492	1497	1500	1501	1502	1508	1514	1515	1517
	1540	1561	1600	1625	1632	1645	1684	1737	3011	3021	3024	3028
	3041	3043	3052	3063	3069	3080	3086	3088	3092	3095	3100	3106
	3110	3118	3150	3156	3159	3160	3165	3167	3169	3179	3179	3181
	3195	3196	3205	3208	3317	3630						
TS22	-293	15	20	25	32	38	42	47	53	57	60	64
	71	71	78	88	93	103	118	124	131	145	148	158
	182	187	193	205	215	220	234	238	242	248	267	269
	280	291	311	317	325	329	349	359	376	404	412	416
	418	425	434	441	448	454	471	481	498	518	526	547
	562	564	589	609	625	627	636	637	649	675	678	691
	700	711	715	737	777	778	793	801	810	816	859	861
	873	885	893	895	899	899	908	936	939	955	963	969

	979 989 992 1002 1003 1005 1021 1023 1027 1029 1032 1053 1056 1057 1057 1064 1070 1071 1076 1097 1104 1104 1114 1131 1133 1156 1164 1172 1179 1183 1187 1196 1214 1219 1222 1237 1251 1269 1293 1301 1313 1317 1331 1336 1340 1341 1357 1360 1387 1391 1394 1397 1399 1405 1411 1417 1420 1423 1425 1459 1467 1472 1474 1482 1483 1485 1485 1485 1488 1493 1494 1499 1500 1502 1511 1515 1525 1532 1532 1566 1612 1625 1629 1645 1719 1725 2851 2970 2983 3021 3023 3027 3028 3028 3034 3052 3067 3086 3087 3088 3089 3094 3099 3103 3104 3108 3117 3151 3157 3157 3163 3165 3172 3178 3179 3181 3185 3186 3195 3203 3204 3206 3585
INT22	12 18 24 31 34 40 43 49 53 60 60 72 77 87 98 105 111 118 130 139 143 150 159 163 168 179 186 200 209 214 225 240 246 254 257 265 272 276 310 321 335 347 354 367 382 395 406 419 431 441 448 456 468 471 486 489 522 531 540 558 560 574 616 634 636 643 652 670 672 694 706 715 718 722 729 744 783 804 815 817 818 839 865 881 889 891 891 908 920 924 931 942 948 971 972 986 989 997 1007 1010 1013 1020 1020 1032 1041 1045 1050 1055 1056 1064 1065 1080 1087 1101 1107 1111 1114 1137 1144 1150 1164 1178 1184 1188 1189 1197 1198 1208 1220 1237 1258 1297 1300 1307 1309 1311 1339 1340 1355 1358 1363 1368 1386 1390 1402 1407 1415 1416 1419 1422 1424 1425 1427 1462 1467 1472 1474 1477 1480 1480 1482 1487 1488 1488 1493 1496 1500 1501 1505 1511 1515 1529 1532 1537 1569 1573 1587 1598 1622 1624 1642 1654 2283 3022 3024 3025 3027 3030 3034 3035 3036 3040 3064 3092 3094 3097 3100 3100 3100 3101 3107 3119 3133 3135 3156 3164 3164 3169 3174 3178 3182 3185 3188 3191 3197 3201 3203 3207 3382
TS23	-103 20 26 29 39 44 46 51 58 63 69 71 79 88 93 98 107 115 122 131 139 149 154 161 163 168 171 187 199 211 218 230 235 243 256 262 271 285 298 308 322 330 349 372 380 388 402 418 431 437 439 446 453 459 466 478 486 515 528 552 566 567 627 631 636 643 655 668 669 695 703 706 718 728 742 782 796 804 809 813 817 833 864 872 884 885 891 891 917 926 935 942 947 957 973 976 985 989 996 1004 1009 1010 1018 1020 1032 1046 1048 1054 1055 1059 1063 1066 1084 1085 1101 1102 1111 1116 1140 1144 1158 1163 1179 1182 1183 1191 1198 1220 1221 1235 1262 1297 1299 1309 1311 1315 1332 1345 1356 1359 1366 1367 1391 1391 1397 1408 1409 1411 1417 1420 1420 1425 1426 1461 1468 1474 1475 1481 1482 1484 1486 1487 1491 1492 1493 1495 1500 1502 1505 1511 1518 1524 1526 1533 1539 1568 1581 1587 1622 1625 1644 1652 2973 3017 3024 3027 3028 3029 3035 3041 3043 3067 3074 3087 3092 3094 3098 3099 3100 3107

	3126 3132 3136 3155 3162 3163 3165 3171 3177 3182 3185 3191 3192 3201 3203 3204 3215 3224 3327
INT23	15 21 26 32 33 35 37 41 44 47 52 55 61 69 76 89 97 101 117 121 134 144 156 163 176 178 180 183 193 213 225 239 240 255 257 264 268 271 282 289 312 324 334 350 374 381 399 417 424 426 435 443 445 449 464 469 486 514 529 531 555 559 578 625 628 636 644 667 669 680 689 692 706 713 719 722 744 783 805 807 816 817 834 862 879 885 891 894 914 919 932 941 944 945 970 983 985 995 1007 1010 1011 1013 1020 1022 1032 1045 1048 1053 1057 1059 1061 1061 1078 1087 1102 1108 1109 1112 1134 1138 1149 1172 1179 1185 1186 1187 1193 1203 1223 1238 1250 1267 1298 1303 1311 1312 1338 1341 1356 1357 1359 1369 1390 1392 1393 1403 1408 1409 1414 1416 1418 1421 1426 1427 1446 1467 1474 1474 1479 1479 1484 1485 1487 1488 1488 1490 1492 1501 1502 1510 1512 1513 1522 1530 1533 1567 1585 1615 1623 1626 1644 1653 2990 3009 3019 3023 3024 3026 3034 3035 3044 3050 3061 3086 3089 3094 3096 3097 3099 3106 3112 3132 3138 3158 3163 3165 3170 3173 3175 3177 3183 3191 3197 3201 3203 3207 3217 3536 3641
TS24	-82 20 28 32 39 44 47 50 55 63 64 68 75 80 89 95 100 111 113 119 132 143 149 154 158 159 178 184 191 200 209 220 232 236 241 255 260 265 279 297 310 340 347 358 369 385 402 418 428 437 44
INT24	13 26 29 37 41 44 48 57 61 67 72 75 84 89 99 107 110 122 127 139 150 158 164 171 178 183 187 189 203 209 214 235 240 245 259 262 265 276 297 311 318 339 345 359 363 390 401 418 419 439 441 447 463 469 476 488 510 528 531 557 561 569 616 621 625 636 638 644 652 664 675 679 690 712 718 719 727 745 784 802 814 824 830 863 880 891 893 904 919 920 925 930 942 945 971 983 989 996 997 1004 1010 1010 1020 1020 1029 1041 1046 1049 1052 1055 1062 1063 1069 1074 1086 1099 1106 1110 1134 1143 1174 1175 1179 1179 1189 1197 1198 1211 1223 1235 1237 1282 1287 1309 1313 1317 1330 1334 1343 1352 1360 1366 1372 1388 1392 1403 1407 1414 1416 1417 1421 1427 1431 1455 1460 1472 1474 1475 1477 1481 1483 1485 1488 1491 1491 1497 1503 1506 1511 1514 1530 1534 1536 1575 1577 1622 1627 1643 1645 1650 1663 1965 3025 3028 3036 3036 3041 3043 3051 3054 3065 3092 3098 3098 3101 3101 3110 3124 3140 3143 3156 3159 3162 3163 3172 3173 3178 3182 3183 3196 3201 3203 3204 3219 3238 3560

TS25	-768	16	28	35	39	46	50	55	62	67	72	73
	80	86	89	103	111	115	118	122	134	138	156	160
	171	182	191	199	204	216	223	226	237	242	251	259
	265	269	275	284	314	322	347	363	368	379	395	418
	421	421	436	442	449	450	469	477	511	519	529	536
	566	573	593	603	622	630	633	637	642	665	675	679
	680	691	694	714	720	729	753	784	805	813	819	844
	865	873	893	899	913	925	928	938	941	945	946	970
	979	990	998	999	1008	1010	1013	1020	1024	1031	1037	1042
	1052	1054	1058	1062	1063	1068	1070	1075	1094	1107	1109	1116
	1169	1173	1179	1187	1194	1198	1222	1223	1238	1256	1291	1303
	1317	1327	1338	1349	1351	1358	1361	1365	1379	1385	1391	1403
	1416	1420	1422	1427	1445	1453	1468	1471	1472	1480	1480	1483
	1487	1488	1491	1492	1499	1499	1507	1511	1517	1530	1536	1567
	1598	1622	1639	1643	1647	1657	1665	1682	3025	3027	3030	3037
	3044	3045	3050	3073	3091	3099	3100	3101	3104	3112	3117	3139
	3150	3154	3161	3165	3170	3174	3178	3180	3182	3199	3204	3205
	3211	3237	3561									
TS21b	-132	43	53	58	60	63	73	82	85	90	95	96
	97	103	110	114	122	124	135	138	143	153	156	166
	171	184	194	195	200	203	207	221	227	237	249	261
	269	272	283	289	299	310	319	326	343	357	367	368
	388	402	423	432	435	440	443	485	495	522	530	533
	561	566	566	611	626	632	635	652	656	668	684	697
	720	730	754	777	786	794	799	810	816	826	838	870
	876	876	878	886	895	903	907	915	949	955	973	996
	1000	1001	1003	1008	1009	1012	1016	1018	1019	1027	1027	1032
	1052	1055	1057	1061	1067	1073	1075	1078	1095	1102	1111	1134
	1159	1169	1173	1188	1189	1192	1194	1196	1209	1232	1243	1257
	1287	1297	1304	1312	1333	1341	1348	1352	1372	1382	1385	1395
	1404	1410	1419	1423	1438	1447	1448	1465	1469	1474	1475	1477
	1483	1491	1493	1493	1495	1499	1506	1509	1514	1517	1520	1520
	1537	1557	1571	1595	1607	1613	1630	1639	2543	2959	2993	3000
	3003	3005	3011	3011	3034	3035	3052	3059	3063	3069	3069	3071
	3088	3090	3096	3112	3116	3123	3129	3132	3133	3136	3144	3144
	3149	3151	3152	3159	3166	3168						