

Mechanistic aspects of ammonia synthesis on Ta₃N₅ surfaces in the presence of intrinsic nitrogen vacancies

Constantinos D. Zeinalipour-Yazdi*

*School of Health, Sport and Bioscience, University of East London, Stratford
Campus, Water Lane, London E15 4LZ, UK*

*Department of Natural Sciences, Faculty of Science and Technology, Middlesex
University, The Burroughs, NW4 4BT, UK*

Figure S1 The Cartesian coordinates of the structure of the various intermediates
in Figure 3

Structure A

Ta1	1.983949231	7.776858157	10.330591732
Ta2	7.240108842	7.776375300	12.005539831
Ta3	8.359465879	2.592739903	10.328290597
Ta4	3.102711595	2.584266744	11.996571962
Ta5	1.388621580	0.539765058	10.276742124
Ta6	6.539655053	0.609300816	11.968422364
Ta7	8.949992870	5.737241400	10.287376442
Ta8	3.792624419	5.806887819	11.988599939
Ta9	1.467813412	4.540073544	10.296990317
Ta10	6.550778477	4.561615276	11.976047767
Ta11	8.868874190	9.731306636	10.289161402
Ta12	3.784573477	9.747693848	11.969621488
Ta13	2.032282920	7.788096477	14.131579643
Ta14	7.211990696	7.795928243	15.937258318
Ta15	8.311563200	2.605903081	14.107281892
Ta16	3.137006943	2.597573892	15.890146852
Ta17	1.354607120	0.603252063	14.105611241
Ta18	6.537435654	0.608584821	15.890606068
Ta19	8.971006919	5.801075022	14.123098546
Ta20	3.796034724	5.804451117	15.948416487
Ta21	1.373811376	4.599330150	14.125619745
Ta22	6.528834737	4.604947477	15.906673666
Ta23	8.960328427	9.780805950	14.118630469
Ta24	3.805997538	9.791728779	15.894116187
Ta25	2.055292258	7.791317408	18.021356488
Ta26	7.177423728	7.861598275	19.743884663
Ta27	8.291004052	2.616734441	17.973868234
Ta28	3.178910076	2.589864047	19.709352070

Ta29	1.377128054	0.647668077	18.031129880
Ta30	6.605670129	0.615766164	19.722652967
Ta31	8.931712282	5.834084199	18.057509869
Ta32	3.657944840	5.795851936	19.811032439
Ta33	1.377857653	4.609000874	18.043617597
Ta34	6.652288271	4.479373022	19.752195484
Ta35	8.968130320	9.765369574	18.037985689
Ta36	3.708300295	9.791192631	19.732057460
N1	8.064550563	7.805519497	10.173881018
N2	2.627439935	7.785311478	12.154721188
N3	2.270470202	2.618176751	10.168828956
N4	7.693165812	2.597329881	12.143807963
N5	0.455753533	6.349012566	9.820806127
N6	3.096017144	6.012866853	10.151119051
N7	5.706485137	6.399849181	11.992487981
N8	8.451217526	5.935821173	12.130505502
N9	9.887028454	1.165546781	9.829314254
N10	7.253203193	0.817615493	10.136283820
N11	4.629613759	1.203877462	11.972376921
N12	1.891077958	0.731328564	12.118299164
N13	0.404504159	9.099913301	10.423492066
N14	3.006007151	9.534564315	10.046010351
N15	5.657959880	9.127106153	11.982510447
N16	8.371681769	9.672122248	12.143255397
N17	9.935817542	3.909132209	10.459571023
N18	7.342761792	4.355821396	10.044716414
N19	4.680578816	3.937839439	11.988240340
N20	1.972659847	4.490822419	12.150765973
N21	7.921975962	7.798038257	14.025872199
N22	2.744711118	7.823708820	16.031595743
N23	2.412891375	2.602848706	13.995467784
N24	7.589802599	2.602527570	15.999742287
N25	0.479326525	6.447269425	14.146887752
N26	3.190714879	5.983494028	14.034858156
N27	5.645260067	6.451019633	15.932850615
N28	8.347164336	5.961352502	16.033163725
N29	9.852806510	1.252364279	14.114536581
N30	7.144890791	0.784032126	13.995832866
N31	4.687650405	1.254357655	15.874406622
N32	1.975497441	0.781603287	16.016252966
N33	0.476998080	9.146997349	14.125288904
N34	3.202195317	9.623319553	13.980550173
N35	5.651571650	9.144671781	15.907437197
N36	8.357028015	9.643835487	16.024241537
N37	9.857763873	3.958968900	14.115566118
N38	7.135905659	4.438849063	13.982826140
N39	4.680133194	3.962969326	15.908151015
N40	1.957867907	4.407209160	16.029474688
N41	7.898019207	7.830780237	17.890127420

N42	2.888576276	7.826229820	19.868048047
N43	2.584185185	2.603102418	17.878791394
N44	7.463925608	2.614981382	19.850594380
N45	0.482200566	6.452861404	18.068940125
N46	3.152208774	5.919322115	17.904415082
N47	2.100839253	4.384321988	19.922513903
N48	8.147176922	5.992157730	19.920060711
N49	9.834143129	1.253844061	17.984090897
N50	7.081072377	0.745377064	17.882291518
N51	4.735439228	1.256614825	19.982610641
N52	2.092565895	0.845347660	19.921161835
N53	0.521633186	9.179285837	18.039052942
N54	3.255686444	9.691552417	17.889774965
N55	5.609474141	9.170428617	19.851443135
N56	8.245983113	9.616507165	19.927355959
N57	9.817455251	3.982644544	18.000565861
N58	7.090609332	4.438469790	17.875285495
N59	4.733496965	4.031039151	20.004953558
N60	5.550388950	6.518451867	19.233992304
N61	5.565875710	6.546099221	20.590190431

Structure B

Ta1	1.982427593	7.772815501	10.319129460
Ta2	7.239676822	7.774165031	11.990320189
Ta3	8.358832110	2.591744791	10.312050769
Ta4	3.102410599	2.581614765	11.982393436
Ta5	1.386655050	0.535477673	10.261787186
Ta6	6.540364591	0.607670633	11.953574023
Ta7	8.949647446	5.734371396	10.272536402
Ta8	3.793015169	5.804599759	11.978069539
Ta9	1.469244415	4.538236614	10.284610766
Ta10	6.550708175	4.558939341	11.962845769
Ta11	8.868372930	9.728422184	10.273274416
Ta12	3.784786386	9.745743229	11.954109614
Ta13	2.037107018	7.784237189	14.120006161
Ta14	7.214641133	7.794560030	15.920248699
Ta15	8.314846109	2.606372289	14.092082557
Ta16	3.143275728	2.596230249	15.874314361
Ta17	1.357181183	0.600805427	14.089970766
Ta18	6.543606081	0.608707278	15.875047961
Ta19	8.975012491	5.799046632	14.108703290
Ta20	3.792743256	5.805920959	15.947684142
Ta21	1.379184105	4.598459619	14.114713520
Ta22	6.529047412	4.607391275	15.893577946
Ta23	8.964304477	9.779032084	14.100643708
Ta24	3.811721699	9.790356180	15.876113337
Ta25	2.071191655	7.786169426	18.016368448
Ta26	7.191900208	7.870555148	19.726412157
Ta27	8.301058051	2.620036366	17.955966697

Ta28	3.183902268	2.580725666	19.689576256
Ta29	1.384609741	0.644928421	18.011164055
Ta30	6.618544507	0.621789093	19.706136469
Ta31	8.944434637	5.833953390	18.041910395
Ta32	3.672822253	5.786194995	19.834780230
Ta33	1.392397229	4.611700956	18.035188615
Ta34	6.664575435	4.483075287	19.739214366
Ta35	8.979880681	9.765258001	18.017538117
Ta36	3.718794396	9.789717592	19.712024410
N1	8.063877879	7.803255876	10.157839863
N2	2.629506054	7.781728736	12.141993074
N3	2.270298098	2.617434097	10.155194417
N4	7.695258338	2.596519228	12.128707539
N5	0.455334677	6.348182995	9.808738834
N6	3.095348215	6.009069157	10.139203368
N7	5.706586471	6.397353408	11.978298424
N8	8.452567042	5.933162002	12.115586683
N9	9.885883850	1.160659640	9.807986672
N10	7.251938689	0.816778459	10.121917212
N11	4.629340550	1.201475651	11.957359043
N12	1.891416980	0.730000308	12.103200131
N13	0.402880911	9.097564670	10.418307686
N14	3.002152918	9.531312898	10.030113143
N15	5.657882016	9.125015205	11.966239090
N16	8.369494200	9.670649709	12.127596341
N17	9.935399674	3.906555574	10.439189641
N18	7.340726952	4.353201388	10.030446932
N19	4.680717201	3.935530922	11.976965103
N20	1.971872778	4.488443383	12.138448867
N21	7.923025234	7.795629361	14.008937675
N22	2.752427439	7.821466023	16.018151262
N23	2.414708701	2.601190262	13.981774004
N24	7.596345973	2.602369297	15.985542934
N25	0.482460886	6.446074779	14.133787296
N26	3.194407641	5.980152715	14.025826948
N27	5.646625393	6.450384355	15.924001282
N28	8.353329377	5.962260259	16.019723156
N29	9.855781296	1.250481334	14.097023889
N30	7.147325572	0.784674278	13.980801202
N31	4.693238718	1.253308923	15.856960806
N32	1.980651009	0.777369228	16.000663681
N33	0.479935140	9.144665776	14.110492031
N34	3.204638746	9.621177738	13.963931898
N35	5.657420147	9.144518491	15.889975592
N36	8.362222433	9.641584135	16.006851754
N37	9.861480443	3.957803137	14.102771037
N38	7.137757384	4.438029788	13.969514558
N39	4.683272393	3.962737888	15.900203602
N40	1.965745980	4.406775445	16.017344902

N41	7.898088962	7.832754179	17.873569398
N42	2.898641100	7.842720733	19.857033279
N43	2.589142234	2.598553655	17.860205299
N44	7.477752029	2.618125644	19.837343458
N45	0.486403027	6.456481700	18.071308795
N46	3.153066572	5.920755587	17.906830484
N47	2.101131785	4.363415836	19.906720616
N48	8.153046063	5.993852321	19.907100690
N49	9.843774375	1.254854515	17.966197525
N50	7.092221404	0.746246943	17.866514191
N51	4.750735828	1.264918826	19.943411370
N52	2.105032003	0.841704694	19.907948530
N53	0.530880924	9.179378231	18.020719292
N54	3.266360160	9.688878033	17.870924633
N55	5.623942082	9.175576419	19.852556252
N56	8.263730669	9.614524132	19.909878564
N57	9.823846781	3.986100217	17.979674895
N58	7.089810699	4.437831707	17.862325088
N59	4.740289039	4.037946157	20.019752500
N60	5.550079079	6.517442150	19.234737348
N61	5.584704075	6.549637327	20.587708249
H1	3.000047377	5.647143172	22.144668684
H2	3.673770075	5.987486659	22.233235995

Structure C

Ta1	1.982355114	7.774893700	10.304692768
Ta2	7.240744793	7.775919386	11.980377727
Ta3	8.360114646	2.594891292	10.298044061
Ta4	3.102388728	2.583718229	11.968493831
Ta5	1.386242232	0.536504901	10.248746814
Ta6	6.540314335	0.609678360	11.939487522
Ta7	8.949144893	5.738178560	10.260122269
Ta8	3.793709649	5.806915584	11.963600827
Ta9	1.469410421	4.540357198	10.271042856
Ta10	6.551316957	4.561247058	11.949461969
Ta11	8.867884867	9.729661808	10.260294679
Ta12	3.785524824	9.747740334	11.939742121
Ta13	2.037224362	7.787867753	14.104832500
Ta14	7.222178710	7.798806018	15.921585753
Ta15	8.317117476	2.610308730	14.076784160
Ta16	3.143945771	2.599498076	15.859037053
Ta17	1.356561790	0.603069653	14.076209416
Ta18	6.543332598	0.610540419	15.858642464
Ta19	8.972829137	5.805559334	14.097854235
Ta20	3.795874007	5.810012809	15.930476866
Ta21	1.377629261	4.602970190	14.100509888
Ta22	6.529795734	4.612670101	15.879808063
Ta23	8.963071141	9.780158613	14.087509643
Ta24	3.813820819	9.792377793	15.861285228

Ta25	2.071888480	7.791877521	18.001686835
Ta26	7.183210053	7.880605336	19.754624624
Ta27	8.307686072	2.625071312	17.933397182
Ta28	3.186992782	2.585316154	19.668947496
Ta29	1.383386612	0.647207340	17.994866819
Ta30	6.631851976	0.636105292	19.687081115
Ta31	8.935629171	5.848716777	18.037455916
Ta32	3.662698611	5.790433178	19.811541532
Ta33	1.385050615	4.619425344	18.016534559
Ta34	6.664914907	4.482741721	19.723688286
Ta35	8.977415486	9.762802998	18.005905333
Ta36	3.719414482	9.801388072	19.698977865
N1	8.064628569	7.804421217	10.145857760
N2	2.630606729	7.784400450	12.127033425
N3	2.270789308	2.619746736	10.141879813
N4	7.696113237	2.599877228	12.114619315
N5	0.455267220	6.350210249	9.794435689
N6	3.095325771	6.011218376	10.124924491
N7	5.707431549	6.399794816	11.965495408
N8	8.453476542	5.935777605	12.103350956
N9	9.886182109	1.161960706	9.793017216
N10	7.253228403	0.818611957	10.108391776
N11	4.629784734	1.203811250	11.942189176
N12	1.891761914	0.732390494	12.090001671
N13	0.402933305	9.099475962	10.407379116
N14	3.001467467	9.533747647	10.014681973
N15	5.658366551	9.127086634	11.953026043
N16	8.369245862	9.672128111	12.114565827
N17	9.935822678	3.908478743	10.426068497
N18	7.341463697	4.356644048	10.016622837
N19	4.681485013	3.937690481	11.962870924
N20	1.972494587	4.490701775	12.124977557
N21	7.921926482	7.797193168	13.999739578
N22	2.752301712	7.825141377	16.003030762
N23	2.414291873	2.603444290	13.968754657
N24	7.598635408	2.606440029	15.970623301
N25	0.482528140	6.449448837	14.119537033
N26	3.195320747	5.984215915	14.010052019
N27	5.648774459	6.455127537	15.915734128
N28	8.352544939	5.966496881	16.008568936
N29	9.855870776	1.252876314	14.085021018
N30	7.148515047	0.787836151	13.965580184
N31	4.693506055	1.256192642	15.838549341
N32	1.982057606	0.777298102	15.987725420
N33	0.480189301	9.147555506	14.095085811
N34	3.206135924	9.623179115	13.948952395
N35	5.659223440	9.146462828	15.880910134
N36	8.360721846	9.642801054	15.991558509
N37	9.861047102	3.961944765	14.090170421

N38	7.138188951	4.441975478	13.955874923
N39	4.683897162	3.966387870	15.883756060
N40	1.965232140	4.411839988	16.003036824
N41	7.906187581	7.836079931	17.879801916
N42	2.900794141	7.841634505	19.841979237
N43	2.585269158	2.601180928	17.844222450
N44	7.480105629	2.617545094	19.822537415
N45	0.487277023	6.461360905	18.059234441
N46	3.158630514	5.925167620	17.889334910
N47	2.101461488	4.375611127	19.889749688
N48	8.149303845	5.984056629	19.898053165
N49	9.847384275	1.260025852	17.946291172
N50	7.096618087	0.747687195	17.846547627
N51	4.752994279	1.271187340	19.893693157
N52	2.111832839	0.840487768	19.898161489
N53	0.535458991	9.184006862	18.009355705
N54	3.275873658	9.689795117	17.858010223
N55	5.630254248	9.183622747	19.895759184
N56	8.270088810	9.643782285	19.888972377
N57	9.822308099	3.992866352	17.964113649
N58	7.092223593	4.442292685	17.847525543
N59	4.738487524	4.042293715	19.995721124
N60	5.557702875	6.531758856	19.231557821
N61	5.581357598	6.538878732	20.581846165
H1	2.967482045	5.653326043	22.194246953
H2	3.643581253	5.983255243	22.284093503
H3	7.279985303	7.690296963	22.206816381
H4	7.817800462	8.216273698	22.109404610

Structure D

Ta1	1.992231507	7.774385901	10.301358177
Ta2	7.251084251	7.776881830	11.977959838
Ta3	8.370638054	2.599463786	10.284527133
Ta4	3.112224344	2.585953559	11.964511824
Ta5	1.395273923	0.534602583	10.244719315
Ta6	6.550065148	0.612437844	11.932645667
Ta7	8.956927475	5.744146695	10.255174517
Ta8	3.805154976	5.808364720	11.959479913
Ta9	1.479596220	4.543212554	10.267900464
Ta10	6.561893361	4.563337647	11.941697038
Ta11	8.877828082	9.731442058	10.250822130
Ta12	3.796243139	9.748646444	11.935443531
Ta13	2.049316815	7.785707906	14.101581555
Ta14	7.269301245	7.794208411	15.943918925
Ta15	8.331098422	2.614520340	14.060049743
Ta16	3.159559106	2.603983547	15.850863680
Ta17	1.369333809	0.598833002	14.069604273
Ta18	6.544978083	0.604389569	15.849902870
Ta19	8.972980933	5.812732162	14.100354483

Ta20	3.818904824	5.815580316	15.925023372
Ta21	1.381318113	4.611610662	14.096168034
Ta22	6.550882168	4.621884304	15.878430044
Ta23	8.972977971	9.784909445	14.071232627
Ta24	3.827312975	9.780812067	15.858993380
Ta25	2.090905039	7.782391396	18.011398156
Ta26	7.244418946	8.053183345	19.927058680
Ta27	8.335085686	2.632515327	17.892802648
Ta28	3.185056996	2.579848287	19.621460732
Ta29	1.395250193	0.628398977	17.969311705
Ta30	6.652524806	0.702740174	19.675312458
Ta31	8.876760472	5.903218746	18.101181360
Ta32	3.583883120	5.723202686	19.807065151
Ta33	1.336853661	4.628984795	17.984089413
Ta34	6.665492626	4.451051359	19.734251708
Ta35	8.995437189	9.756356643	17.963993870
Ta36	3.712550392	9.805964201	19.714161797
N1	8.076338155	7.804985266	10.140287270
N2	2.641398633	7.783804235	12.121968832
N3	2.282982020	2.623062078	10.141391283
N4	7.712056055	2.606584270	12.102971405
N5	0.465124987	6.354782981	9.796949813
N6	3.104220566	6.010690393	10.120169611
N7	5.717452028	6.402807784	11.958744477
N8	8.462032653	5.936774735	12.098292851
N9	9.896857650	1.160737277	9.779312048
N10	7.263897318	0.821687457	10.101577914
N11	4.639895355	1.205209337	11.938294170
N12	1.904799857	0.734678327	12.086989716
N13	0.412002117	9.102560372	10.413316862
N14	3.008402434	9.535695409	10.009348225
N15	5.669565592	9.129840832	11.945320607
N16	8.377010034	9.674755208	12.105664389
N17	9.945483475	3.910092961	10.409735559
N18	7.349620249	4.360808216	10.009249338
N19	4.691865593	3.939388649	11.957403261
N20	1.980170052	4.491134218	12.123105394
N21	7.927478065	7.798978961	13.998501319
N22	2.765971616	7.819857260	15.998300409
N23	2.422946641	2.606374471	13.972366414
N24	7.619916693	2.625102090	15.964270338
N25	0.490486203	6.451979487	14.120984389
N26	3.210659588	5.985477519	14.003889399
N27	5.668844676	6.465596693	15.940880588
N28	8.352695252	5.961021019	15.999996338
N29	9.868805061	1.255369148	14.077906764
N30	7.159494192	0.798704167	13.957063186
N31	4.701348032	1.254686065	15.829125579
N32	2.006337056	0.755884606	15.978614484

N33	0.490167772	9.148601210	14.082539265
N34	3.221817933	9.616722968	13.943172182
N35	5.680586001	9.144343069	15.888861701
N36	8.366047524	9.647782018	15.971647879
N37	9.869790215	3.965715298	14.079021371
N38	7.143202340	4.442883166	13.950321101
N39	4.697614047	3.970714760	15.868277826
N40	1.971765008	4.429915838	16.004317588
N41	8.008721205	7.822995541	17.905904289
N42	2.910183855	7.819937398	19.843106102
N43	2.555276688	2.585140596	17.820273390
N44	7.497214513	2.611329785	19.830843407
N45	0.501615269	6.452324290	18.084492057
N46	3.215816815	5.927676357	17.893642921
N47	2.075695577	4.363389377	19.893843770
N48	8.106286864	5.933916180	19.920136801
N49	9.871990364	1.266413022	17.898656160
N50	7.098733424	0.761344525	17.827061806
N51	4.752493870	1.260164734	19.791988355
N52	2.138084132	0.789878246	19.890433859
N53	0.553073916	9.175187403	17.979058860
N54	3.316693234	9.664934200	17.864217108
N55	5.669089283	9.219439894	20.132908837
N56	8.315253925	9.753286523	19.841709254
N57	9.820164129	3.989352053	17.944048677
N58	7.109945798	4.468016384	17.860407802
N59	4.713914755	4.001986199	19.762828550
N60	5.603998780	6.601246673	19.609367895
N61	5.390171698	6.242748816	20.928005510
H1	2.524973510	5.553882321	22.547729010
H2	3.182337041	5.843079608	22.764177449
H3	5.773598003	6.883103087	21.651557200
H4	7.706298664	7.863816326	21.650990179

Structure E

Ta1	2.021739722	7.771283236	10.274742321
Ta2	7.250975894	7.782067305	11.993948170
Ta3	8.358413628	2.598791251	10.262744774
Ta4	3.126138303	2.586544710	11.976735269
Ta5	1.464189485	0.602632484	10.225003207
Ta6	6.567798450	0.616446968	11.929908904
Ta7	8.906644822	5.804089590	10.245717638
Ta8	3.801330036	5.813859229	11.974364863
Ta9	1.483922168	4.560410246	10.247153899
Ta10	6.561268350	4.566411726	11.944325809
Ta11	8.896268913	9.743631508	10.231458151
Ta12	3.807111628	9.750773719	11.930925134
Ta13	2.065018684	7.769092391	14.101125449
Ta14	7.264359296	7.790175564	15.941360383

Ta15	8.344315379	2.608840056	14.060647988
Ta16	3.184309321	2.600302088	15.841043728
Ta17	1.382709474	0.587810998	14.062006082
Ta18	6.567652463	0.604703856	15.844198791
Ta19	8.982830565	5.793441749	14.096221083
Ta20	3.777027249	5.828940897	15.992983890
Ta21	1.398439807	4.608286263	14.091443855
Ta22	6.523795820	4.633365204	15.864202132
Ta23	8.993399015	9.775653836	14.069512974
Ta24	3.843897160	9.778157393	15.845759384
Ta25	2.131730199	7.753987169	18.049642990
Ta26	7.232205290	7.935681564	19.863056897
Ta27	8.357028541	2.626919868	17.886961637
Ta28	3.196461277	2.538613925	19.641118931
Ta29	1.406255411	0.617720303	17.949444439
Ta30	6.699270230	0.680776975	19.675015130
Ta31	8.953604867	5.868661433	18.049809401
Ta32	3.573211820	5.668169608	20.077168764
Ta33	1.407898310	4.616502038	17.999550754
Ta34	6.684709368	4.476559911	19.711326699
Ta35	9.006766847	9.739808508	17.976964313
Ta36	3.737077398	9.778498060	19.674965008
N1	8.087132044	7.781575005	10.130214747
N2	2.631154206	7.775716164	12.103764588
N3	2.283581162	2.595408209	10.126098381
N4	7.738073740	2.595994176	12.087157355
N5	0.450954607	6.413246941	9.986340490
N6	3.088615883	5.999336016	10.075668367
N7	5.702803121	6.415886758	11.967623027
N8	8.448509237	5.916297909	12.094396164
N9	9.926354798	1.222965591	9.978611885
N10	7.294546802	0.810167982	10.054009241
N11	4.668753130	1.219636416	11.939288673
N12	1.936605455	0.705407166	12.071443224
N13	0.440982778	9.129298910	10.069206489
N14	3.071659724	9.547721634	10.039520177
N15	5.701902023	9.145506951	11.945173127
N16	8.433864166	9.657255744	12.082502109
N17	9.935849785	3.937981480	10.090068200
N18	7.306472069	4.376907585	10.044243585
N19	4.674549455	3.953589543	11.961932361
N20	1.946248616	4.478536568	12.097018376
N21	7.923575016	7.791636263	13.982979631
N22	2.783629776	7.794654412	15.987986428
N23	2.421867531	2.592670795	13.942148059
N24	7.629204406	2.601079421	15.950390830
N25	0.495864169	6.442714364	14.105702947
N26	3.220613561	5.967110641	13.993710521
N27	5.654439310	6.463605165	15.964973803

N28	8.353304409	5.953266555	15.982331217
N29	9.881221533	1.242283631	14.063963248
N30	7.173084664	0.776674390	13.934010089
N31	4.720842744	1.245460304	15.788162810
N32	2.009295221	0.749715053	15.954778611
N33	0.500888142	9.133001658	14.072797305
N34	3.222016761	9.596053663	13.934184062
N35	5.694239173	9.140685012	15.882136769
N36	8.384858686	9.630898551	15.969005503
N37	9.881953411	3.954706814	14.081326469
N38	7.155340454	4.421416115	13.942043712
N39	4.691657747	3.970482155	15.839623657
N40	2.001771527	4.420218546	15.985303351
N41	7.991417296	7.807377901	17.891607482
N42	2.919458138	7.922815481	19.856939571
N43	2.643477012	2.548703419	17.795601142
N44	7.523946879	2.612787637	19.813076412
N45	0.510803353	6.447400677	18.128038938
N46	3.190994347	5.931138357	17.962492568
N47	2.054320630	4.226203728	19.834248549
N48	8.174556923	5.870093370	19.858293903
N49	9.877452621	1.253555873	17.913709428
N50	7.116189466	0.747491222	17.822708439
N51	4.803272495	1.268723379	19.878613910
N52	2.148490697	0.801999877	19.866423738
N53	0.563642288	9.169007568	17.974968843
N54	3.315895144	9.662105250	17.822737860
N55	5.662348283	9.162921281	19.970282545
N56	8.295646349	9.700837745	19.861874435
N57	9.833077951	3.991217219	17.867454920
N58	7.013078871	4.431403865	17.837546051
N59	4.724837725	4.015665500	20.128594469
N60	5.671030910	6.463272137	20.240413308
N61	4.932034101	6.619068052	21.465969568
H1	2.633408983	5.787516784	21.577870039
H2	5.360660525	6.157565598	22.272732432
H3	4.763067578	7.611165622	21.666558053
H4	7.785719100	7.810609509	21.557767134

Structure F

Ta1	2.033198558	7.776760973	10.292709741
Ta2	7.291564809	7.779250961	11.968647300
Ta3	8.413128041	2.596187349	10.278217618
Ta4	3.151282670	2.586735188	11.958539540
Ta5	1.436568329	0.535437882	10.237298691
Ta6	6.591948962	0.613075977	11.927119531
Ta7	9.000764753	5.742571527	10.242161101
Ta8	3.844424011	5.810224239	11.950390582
Ta9	1.522039065	4.543216978	10.260115477

Ta10	6.599799175	4.564108615	11.924490240
Ta11	8.917227311	9.731126666	10.248207671
Ta12	3.836476145	9.750963451	11.930602726
Ta13	2.090221990	7.788050580	14.092867001
Ta14	7.300469520	7.794911525	15.931770301
Ta15	8.372247637	2.608784346	14.054653460
Ta16	3.200967284	2.603154152	15.845920970
Ta17	1.402065439	0.596742241	14.062542719
Ta18	6.591703261	0.603561122	15.848008985
Ta19	9.028521252	5.807049077	14.077777979
Ta20	3.842762920	5.818682449	15.923712995
Ta21	1.433264168	4.601451965	14.092800717
Ta22	6.577173158	4.626088108	15.839933522
Ta23	9.005518584	9.775149897	14.080307083
Ta24	3.869613108	9.786865710	15.851197398
Ta25	2.128525513	7.788193749	18.001548467
Ta26	7.144310549	7.831573279	19.866643764
Ta27	8.380984880	2.624105393	17.889002896
Ta28	3.202858795	2.565756573	19.654604532
Ta29	1.408679609	0.621823428	17.957085315
Ta30	6.727730724	0.702518006	19.681677354
Ta31	8.991494534	5.881254729	18.029174361
Ta32	3.805061298	5.717967893	19.812264322
Ta33	1.431431240	4.605155087	18.014430410
Ta34	6.742537620	4.549704820	19.672235234
Ta35	8.983653898	9.728744898	18.022760243
Ta36	3.722252620	9.761776332	19.690875022
N1	8.116214973	7.809594722	10.130322609
N2	2.683093105	7.782090128	12.113921120
N3	2.322718942	2.625058722	10.132154247
N4	7.751626421	2.602098364	12.095142078
N5	0.506225061	6.355477660	9.780651206
N6	3.144651691	6.011710457	10.110421540
N7	5.758157412	6.402725242	11.944691442
N8	8.504922268	5.941377830	12.084874753
N9	9.938250302	1.163735619	9.774745951
N10	7.304140806	0.819225317	10.094265429
N11	4.680513813	1.206699933	11.933153703
N12	1.943205560	0.735902665	12.078275522
N13	0.453881673	9.102601183	10.400690338
N14	3.050983024	9.536042946	10.002498336
N15	5.709466819	9.130829505	11.940598072
N16	8.420594031	9.675270023	12.102742150
N17	9.986713233	3.912209755	10.406051740
N18	7.393121283	4.358275386	9.995496417
N19	4.731677421	3.939597339	11.946200714
N20	2.022270634	4.494704059	12.114957352
N21	7.963802730	7.802086098	13.988819683
N22	2.804872538	7.812586344	15.989291323

N23	2.457896370	2.608095151	13.960052645
N24	7.651972843	2.625111901	15.953016598
N25	0.537152530	6.448884298	14.099601749
N26	3.253978915	5.983955096	13.997851293
N27	5.703406850	6.464419602	15.924860438
N28	8.406917671	5.968061584	15.980601346
N29	9.903870335	1.251270641	14.072532631
N30	7.200796401	0.792471614	13.953690466
N31	4.742477063	1.252423038	15.813052799
N32	2.025809953	0.771563847	15.970961523
N33	0.526669173	9.144955974	14.084483148
N34	3.254768044	9.620180990	13.935275939
N35	5.714802944	9.142439319	15.884299709
N36	8.402699873	9.637986468	15.983769442
N37	9.914988395	3.962811904	14.079209124
N38	7.187746995	4.443564998	13.926801758
N39	4.736818499	3.969535576	15.845523810
N40	2.031313524	4.430085433	16.001403941
N41	8.014465227	7.807392553	17.907554595
N42	2.932276750	7.888040044	19.834553283
N43	2.641666207	2.584326293	17.820928702
N44	7.532412533	2.627053993	19.791420805
N45	0.565595454	6.442896364	18.076627519
N46	3.267233208	5.938595908	17.913427370
N47	2.126546983	4.305567942	19.891330675
N48	8.255055886	5.899775124	19.884639321
N49	9.889038637	1.254253634	17.921344722
N50	7.142262193	0.756500109	17.825126079
N51	4.811252409	1.270992300	19.949424072
N52	2.159684622	0.818112222	19.883594467
N53	0.575155916	9.172161863	18.009926538
N54	3.323421886	9.682748803	17.833006670
N55	5.633496701	9.170399738	19.950790187
N56	8.259730082	9.717772735	19.877037335
N57	9.882834413	3.986829638	17.917195745
N58	7.124866896	4.484765685	17.819886760
N59	4.802905119	3.967175472	19.962289649
N60	5.628959202	6.477703656	19.924497993
N61	3.321527525	6.099873252	22.044994102
H1	2.311634332	6.243887142	22.128853620
H2	3.594240737	5.342107787	22.675877289
H3	3.791721525	6.960110646	22.337775240
H4	7.649360792	7.804299326	21.579833501

Structure G

Ta1	1.980588088	7.786200757	10.318186182
Ta2	7.239710141	7.780799159	11.994974915
Ta3	8.358624919	2.594274778	10.306208560
Ta4	3.098736604	2.589420474	11.991472479

Ta5	1.386527565	0.544150010	10.273338758
Ta6	6.538256297	0.614491825	11.955793233
Ta7	8.947634121	5.744683338	10.266945030
Ta8	3.794125633	5.811644529	11.967951523
Ta9	1.464598628	4.545034500	10.285532243
Ta10	6.549570342	4.565271512	11.949724927
Ta11	8.865762566	9.734651505	10.277283942
Ta12	3.783129079	9.753289406	11.964772345
Ta13	2.028923668	7.802128542	14.115299884
Ta14	7.251539157	7.799701739	15.958072704
Ta15	8.315539494	2.609541467	14.083960316
Ta16	3.141529075	2.607349848	15.888231914
Ta17	1.351038105	0.607979529	14.104568809
Ta18	6.537464777	0.604339496	15.881126407
Ta19	8.971320672	5.813219970	14.103014507
Ta20	3.816646634	5.810656794	15.903865367
Ta21	1.371730144	4.605552248	14.113243339
Ta22	6.540587757	4.620180951	15.871470039
Ta23	8.949977004	9.782305632	14.111135465
Ta24	3.813644438	9.796135693	15.895320779
Ta25	2.044781099	7.813924546	17.995974063
Ta26	7.064053069	7.811734938	19.902221482
Ta27	8.312713545	2.620912928	17.933231081
Ta28	3.165498673	2.619476612	19.703034715
Ta29	1.355466389	0.642512481	18.017591592
Ta30	6.662702058	0.690758444	19.715042272
Ta31	8.916489581	5.887912270	18.065187224
Ta32	3.667834314	5.832802400	19.744021889
Ta33	1.353747982	4.599222852	18.019724415
Ta34	6.661503058	4.549426149	19.712287548
Ta35	8.918748531	9.735555682	18.065713861
Ta36	3.668791444	9.793407706	19.742889763
N1	8.064224135	7.810926500	10.159349194
N2	2.626855794	7.794014971	12.141001691
N3	2.268039901	2.621867934	10.165110963
N4	7.697761140	2.600861025	12.123609592
N5	0.453540150	6.355375822	9.808113732
N6	3.090175893	6.018877348	10.135093542
N7	5.707284625	6.403909444	11.967541762
N8	8.449864867	5.941525130	12.110150455
N9	9.884970110	1.166890993	9.812681676
N10	7.248910147	0.819871694	10.122473224
N11	4.627424626	1.209911846	11.966896533
N12	1.888647046	0.737925225	12.116626884
N13	0.401684129	9.104593574	10.424526441
N14	3.000772034	9.545724188	10.037085872
N15	5.655545510	9.132208056	11.972822413
N16	8.367632798	9.678572961	12.131727352
N17	9.933325940	3.913371848	10.437476240

N18	7.340673081	4.358319010	10.023711734
N19	4.679114433	3.942318748	11.970277013
N20	1.970123538	4.496619219	12.140630511
N21	7.917686382	7.804612637	14.015278080
N22	2.738373450	7.820045004	16.020374205
N23	2.407937072	2.611937147	13.996630727
N24	7.596008790	2.626361607	15.984889307
N25	0.483061319	6.452450539	14.121882785
N26	3.198411488	5.996598396	14.007617578
N27	5.661327058	6.466670370	15.924527971
N28	8.350785019	5.967444887	16.004663048
N29	9.850605813	1.257112375	14.105548872
N30	7.144677891	0.794355288	13.984713982
N31	4.687049473	1.257788119	15.862640718
N32	1.971631560	0.785603818	16.016228232
N33	0.473549832	9.153385418	14.119435587
N34	3.203546496	9.627218860	13.976900016
N35	5.657573116	9.145205416	15.922752435
N36	8.347972543	9.642555060	16.011933620
N37	9.859972358	3.965074079	14.104222574
N38	7.138803511	4.443483297	13.954005339
N39	4.690684599	3.969873207	15.861361655
N40	1.975581525	4.440839325	16.023245726
N41	7.958513699	7.808275726	17.933640883
N42	2.897657715	7.814349318	19.853986100
N43	2.575706051	2.615538945	17.868415287
N44	7.455643756	2.621116441	19.819235090
N45	0.521956605	6.443008031	18.047661107
N46	3.259893412	5.937380776	17.888919973
N47	2.103538098	4.396286698	19.920434441
N48	8.196813856	5.903492672	19.907253976
N49	9.828526844	1.257392806	17.968555314
N50	7.090882288	0.751878210	17.857503477
N51	4.740415230	1.266033074	19.957171452
N52	2.103417306	0.843087740	19.921486609
N53	0.522567582	9.181206364	18.052541429
N54	3.265814226	9.693427736	17.886873396
N55	5.565235837	9.166813655	19.978474180
N56	8.197002084	9.717104859	19.906777533
N57	9.828751975	3.980865380	17.972667052
N58	7.086510393	4.492474577	17.854225691
N59	4.738266203	3.977874833	19.954276555
N60	5.563506655	6.460091184	19.976555716
H1	7.587578808	7.807258309	21.598832878

Structure H

Ta1	1.989131850	7.789255272	10.295596317
Ta2	7.247729549	7.785369359	11.974125666
Ta3	8.367095791	2.598618776	10.285177142

Ta4	3.106815337	2.594135049	11.967332443
Ta5	1.394053140	0.546835342	10.249615062
Ta6	6.547053212	0.618484792	11.934494635
Ta7	8.955500358	5.749089540	10.246051837
Ta8	3.802263473	5.816094936	11.945573164
Ta9	1.472860715	4.550095385	10.263183919
Ta10	6.557727310	4.569242213	11.929566964
Ta11	8.874115471	9.738316917	10.255987979
Ta12	3.791474162	9.758410642	11.941048537
Ta13	2.038358802	7.802567649	14.092262942
Ta14	7.259713944	7.800702203	15.936932610
Ta15	8.324552133	2.611044074	14.063571545
Ta16	3.151585859	2.609124994	15.863196613
Ta17	1.359816846	0.609319929	14.080200922
Ta18	6.546429957	0.605183731	15.859946465
Ta19	8.980107525	5.814612184	14.081844608
Ta20	3.822164557	5.812801152	15.886249658
Ta21	1.381010762	4.607462440	14.091191526
Ta22	6.547622576	4.622929223	15.850209515
Ta23	8.959078261	9.783577266	14.090159191
Ta24	3.822657605	9.796952216	15.870399433
Ta25	2.058291039	7.810741832	17.974416435
Ta26	7.075721393	7.814352084	19.880691774
Ta27	8.323996528	2.621269259	17.910461075
Ta28	3.175207059	2.616223815	19.676384124
Ta29	1.365450284	0.639784581	17.991447688
Ta30	6.673144644	0.691657773	19.693092598
Ta31	8.928250464	5.888034088	18.043246460
Ta32	3.681195075	5.826871032	19.732259677
Ta33	1.365568634	4.599012419	17.999067455
Ta34	6.672603441	4.549918293	19.687824533
Ta35	8.929635442	9.734148167	18.043542145
Ta36	3.678277437	9.789653632	19.717179603
N1	8.072136963	7.815425047	10.137563797
N2	2.636632910	7.796487768	12.117772006
N3	2.276531445	2.628043546	10.141695623
N4	7.707228309	2.604415289	12.102881671
N5	0.460991193	6.360990206	9.787074245
N6	3.099048924	6.022828327	10.111676377
N7	5.715629035	6.408137558	11.947842615
N8	8.458589462	5.946109673	12.089208219
N9	9.893428045	1.170675532	9.788679150
N10	7.257831820	0.824080551	10.101540926
N11	4.636433443	1.214341696	11.944150881
N12	1.897860812	0.742597726	12.092557706
N13	0.410356168	9.109321539	10.406418985
N14	3.008395940	9.548926363	10.012844020
N15	5.663765245	9.136485571	11.949737341
N16	8.376300460	9.682463109	12.110424852

N17	9.941368521	3.918175645	10.414228403
N18	7.348103336	4.362166738	10.003503438
N19	4.687136774	3.946650390	11.947752111
N20	1.978208575	4.501301737	12.117983495
N21	7.924380829	7.807438898	13.993776364
N22	2.749134465	7.820156487	15.996303064
N23	2.415875505	2.614962905	13.972842469
N24	7.605377611	2.627569641	15.964251259
N25	0.491417521	6.454849751	14.101624712
N26	3.207172929	5.997792692	13.986465917
N27	5.668795579	6.467742453	15.906370751
N28	8.360466311	5.969886313	15.983577144
N29	9.859324751	1.258929054	14.086145446
N30	7.153601177	0.796648696	13.963846732
N31	4.696524951	1.258649070	15.840085033
N32	1.981347296	0.785612994	15.991341798
N33	0.482333609	9.155239159	14.095760758
N34	3.212083321	9.629375622	13.952352782
N35	5.666441244	9.146127832	15.897822173
N36	8.357513043	9.642613367	15.991024719
N37	9.868967988	3.967388590	14.082068932
N38	7.147345884	4.445883827	13.933519691
N39	4.699160339	3.971278591	15.839203300
N40	1.984722125	4.441353926	16.001013926
N41	7.968081349	7.808571081	17.912285146
N42	2.908967860	7.818633783	19.829328989
N43	2.585979964	2.613455614	17.842840246
N44	7.465908251	2.621839407	19.797244756
N45	0.531781664	6.442478835	18.030012782
N46	3.267405991	5.936257794	17.872778613
N47	2.110874769	4.388717862	19.898307034
N48	8.207210094	5.904033292	19.886124627
N49	9.839351202	1.256880016	17.945675419
N50	7.101494683	0.750523644	17.836048633
N51	4.751899009	1.266269914	19.930571231
N52	2.115265145	0.839653646	19.896794418
N53	0.532971688	9.179685546	18.028244776
N54	3.276475707	9.691900853	17.860898635
N55	5.575647465	9.167365838	19.963450322
N56	8.207729502	9.715549189	19.886047981
N57	9.839073177	3.980866349	17.950448903
N58	7.097189944	4.493286812	17.831247720
N59	4.748153750	3.978603969	19.927102449
N60	5.575151880	6.461789308	19.949396410
H1	7.592919167	7.801541036	21.581011110
H2	3.507429142	5.808976345	22.538592052
H3	4.168932866	6.146151240	22.412199134

Structure I

Ta1	1.990038476	7.780051367	10.306662844
Ta2	7.241556751	7.785168144	11.984004637
Ta3	8.362759600	2.605296421	10.290484094
Ta4	3.103930970	2.593956995	11.972404033
Ta5	1.392534631	0.546353965	10.245283469
Ta6	6.546246849	0.620102767	11.940076697
Ta7	8.949601076	5.751758048	10.259807643
Ta8	3.796557307	5.815920506	11.973297247
Ta9	1.476868742	4.551724279	10.273427030
Ta10	6.552162102	4.569390069	11.947506029
Ta11	8.874092850	9.736457845	10.259265567
Ta12	3.790303045	9.759423594	11.939988338
Ta13	2.047806862	7.790081566	14.106093775
Ta14	7.249231175	7.796756308	15.938287753
Ta15	8.324089834	2.619068014	14.070331183
Ta16	3.163367499	2.606644605	15.858409399
Ta17	1.359210584	0.603856623	14.068811025
Ta18	6.538187080	0.609695635	15.858302606
Ta19	8.977032335	5.809987888	14.097701368
Ta20	3.780104514	5.842389287	15.968327880
Ta21	1.387052988	4.613872754	14.107076544
Ta22	6.522448309	4.633815484	15.872782353
Ta23	8.966427281	9.786003597	14.083835868
Ta24	3.815605211	9.781613323	15.858853372
Ta25	2.106489945	7.791410755	18.049583750
Ta26	7.168774019	7.911388652	19.873315331
Ta27	8.341241701	2.626428141	17.895973547
Ta28	3.171682241	2.532074055	19.653980540
Ta29	1.378216794	0.625504325	17.958479092
Ta30	6.678252213	0.682188166	19.686635795
Ta31	8.921634845	5.886935066	18.058228070
Ta32	3.634730663	5.617021046	19.930437218
Ta33	1.366965265	4.636502629	18.002963337
Ta34	6.724551013	4.476942192	19.735996730
Ta35	8.969148691	9.740302896	17.990968998
Ta36	3.677643744	9.754541440	19.707588163
N1	8.071627925	7.811956419	10.146836651
N2	2.642546186	7.786104285	12.127156588
N3	2.278246315	2.632239046	10.145564135
N4	7.708907335	2.608937773	12.110323217
N5	0.458133651	6.368312626	9.813271499
N6	3.096911316	6.013533394	10.126968610
N7	5.708770058	6.409580756	11.964929694
N8	8.455067566	5.941960682	12.103653632
N9	9.891604532	1.170943241	9.791514643
N10	7.258790305	0.826720003	10.107860463
N11	4.635537863	1.215121858	11.944771259
N12	1.897720675	0.746599366	12.086802706

N13	0.409349221	9.110784701	10.410186450
N14	3.004465298	9.542900110	10.015114420
N15	5.664419810	9.138410326	11.951137734
N16	8.375292431	9.681627621	12.114169230
N17	9.938191995	3.918544425	10.399007691
N18	7.340076637	4.366149065	10.018023952
N19	4.682681994	3.946703478	11.967856159
N20	1.967477287	4.499294882	12.129247182
N21	7.912543051	7.807164155	14.001055060
N22	2.774362060	7.827551786	15.988256792
N23	2.409054516	2.619309975	13.977061960
N24	7.609463519	2.631959691	15.972257805
N25	0.486336681	6.456772902	14.122432452
N26	3.203969546	5.981371972	14.019418823
N27	5.649472122	6.473900932	15.962384352
N28	8.343959629	5.966058977	15.995787583
N29	9.858094730	1.258150097	14.086657673
N30	7.154217293	0.800393363	13.968050231
N31	4.696028451	1.260261374	15.820659795
N32	1.986299736	0.767527010	15.974939983
N33	0.481418023	9.151557668	14.086020850
N34	3.206639957	9.631569448	13.939652237
N35	5.669856766	9.151099827	15.890165755
N36	8.362117876	9.640662963	15.991955166
N37	9.867173450	3.969685001	14.092983353
N38	7.132576202	4.444236002	13.952310461
N39	4.681272510	3.983341104	15.872697261
N40	1.977726586	4.445023826	16.024053470
N41	7.965344635	7.807863386	17.912658855
N42	2.837267591	7.959081180	19.868309851
N43	2.597028324	2.568403833	17.827087666
N44	7.516364657	2.607729456	19.829078996
N45	0.497723425	6.446335225	18.108029913
N46	3.201126515	5.986317498	17.953066727
N47	2.090190008	4.296599782	19.892480679
N48	8.177316562	5.904943578	19.892136738
N49	9.847735386	1.255953518	17.926931179
N50	7.093374355	0.762124620	17.837909886
N51	4.778261231	1.284445402	19.909150810
N52	2.114457738	0.810518700	19.886709508
N53	0.525891209	9.177347830	17.985478450
N54	3.280211776	9.678981658	17.842136142
N55	5.607776536	9.164415140	19.931969549
N56	8.234872785	9.692723990	19.879013220
N57	9.829411166	3.990034652	17.911974984
N58	7.047416380	4.471638975	17.864055339
N59	4.766645732	3.973718951	19.972058544
N60	5.592595847	6.459117866	20.298921306
H1	7.741003340	7.839473489	21.556248999

H2	3.219101328	6.087967382	21.616913573
H3	5.467041915	6.631415661	21.314367786

Structure J

Ta1	1.985388669	7.768733414	10.306026937
Ta2	7.250506806	7.763650764	11.975476574
Ta3	8.358089244	2.587255985	10.272363076
Ta4	3.096797613	2.581803092	11.974699567
Ta5	1.393493334	0.538702750	10.253163675
Ta6	6.539637563	0.597557450	11.915563747
Ta7	8.934474703	5.750187472	10.249157270
Ta8	3.794447947	5.803010017	11.958320685
Ta9	1.454908926	4.538233045	10.275751717
Ta10	6.547697927	4.550764963	11.929398638
Ta11	8.873211929	9.721134750	10.244423605
Ta12	3.790880178	9.740267437	11.938028094
Ta13	2.035052082	7.777031510	14.107840882
Ta14	7.262919081	7.791268723	15.946112752
Ta15	8.329195130	2.593993876	14.038018846
Ta16	3.146132523	2.597207071	15.868797809
Ta17	1.354640653	0.595675653	14.075256789
Ta18	6.539042060	0.590671446	15.823262651
Ta19	8.967406182	5.809439764	14.091177962
Ta20	3.804732872	5.811915251	15.930967830
Ta21	1.371699216	4.590408682	14.106304365
Ta22	6.531345480	4.597032033	15.847125525
Ta23	8.958447736	9.756596904	14.072391424
Ta24	3.819590681	9.773890737	15.857079518
Ta25	2.040336019	7.804145686	18.013526135
Ta26	7.110503239	7.930651961	19.925403946
Ta27	8.359333788	2.542837171	17.857094623
Ta28	3.188734684	2.564604282	19.678675568
Ta29	1.379444151	0.628471248	17.968812529
Ta30	6.631694874	0.610883005	19.648212202
Ta31	8.839620088	5.843410800	18.037782167
Ta32	3.549786544	5.775657178	19.843632071
Ta33	1.336285131	4.627854267	18.008841534
Ta34	6.743179227	4.274046323	19.680350072
Ta35	8.936133360	9.695498247	18.001066572
Ta36	3.656869872	9.809738435	19.696401297
N1	8.073764381	7.779064010	10.130247913
N2	2.623335050	7.774019530	12.132792072
N3	2.266681789	2.606013183	10.151483458
N4	7.695058773	2.586599239	12.090091157
N5	0.457234322	6.345511065	9.816300747
N6	3.101261777	6.008937906	10.123500799
N7	5.711143747	6.391170860	11.958780578
N8	8.454550515	5.913406306	12.098059530
N9	9.889737578	1.155082014	9.799641713

N10	7.255078010	0.802945270	10.084086605
N11	4.629272053	1.196330358	11.939635168
N12	1.894562693	0.718966249	12.100021713
N13	0.407664740	9.092275410	10.379703426
N14	3.010937840	9.529259012	10.024927142
N15	5.663415549	9.115441021	11.939602668
N16	8.376360656	9.658417691	12.099764775
N17	9.931938890	3.894461297	10.382147353
N18	7.333179950	4.351931333	10.005745644
N19	4.674568917	3.931132852	11.956002647
N20	1.962241137	4.496559354	12.132773037
N21	7.922339193	7.778905370	14.005532494
N22	2.742801463	7.805552679	16.020574344
N23	2.403304186	2.608848624	13.987416701
N24	7.619479552	2.573368662	15.935261059
N25	0.479760244	6.440820284	14.120840035
N26	3.211451988	5.982923233	14.019781137
N27	5.669363199	6.442048724	15.953805063
N28	8.356619038	5.932845126	16.021800663
N29	9.856228328	1.237224711	14.070099258
N30	7.148703533	0.769289578	13.938774674
N31	4.689105696	1.241824537	15.825620842
N32	1.984372626	0.769096817	15.992210442
N33	0.479765769	9.137860999	14.100036951
N34	3.211659721	9.604442654	13.956242018
N35	5.666052138	9.121973549	15.888284432
N36	8.358810182	9.630039090	15.988483512
N37	9.863400886	3.952762139	14.092248866
N38	7.136590146	4.421045310	13.940240101
N39	4.681314581	3.960554723	15.855205310
N40	1.963264622	4.449951372	16.041148903
N41	7.977366847	7.799674521	17.939293479
N42	2.850759110	7.880005281	19.865042129
N43	2.606528427	2.614401929	17.860991659
N44	7.591772462	2.494129193	19.812658133
N45	0.462852804	6.431749961	18.071579019
N46	3.268965624	5.954009892	17.944342303
N47	2.118034726	4.399741151	19.974033912
N48	7.863844826	5.912311519	19.887842887
N49	9.852004364	1.215266839	17.887616870
N50	7.082007200	0.721260994	17.810408198
N51	4.741740154	1.284128652	19.966891490
N52	2.091697178	0.869475645	19.892065703
N53	0.520406119	9.166401015	18.027249480
N54	3.252075111	9.688851135	17.853079737
N55	5.570379602	9.155052298	19.770506309
N56	8.204505510	9.669459493	19.902680963
N57	9.829553490	3.963415409	17.995746858
N58	7.099213324	4.354753154	17.810629998

N59	4.800817716	4.205557111	19.896877133
N60	5.262052454	6.759954108	20.995614247
H1	7.669654953	7.942549333	21.614835275
H2	4.880157965	7.564082129	21.503217198
H3	5.683614334	6.164999707	21.716741150

Structure K

Ta1	1.954963620	7.751817730	10.283750841
Ta2	7.212214135	7.759196077	11.964191462
Ta3	8.329373740	2.589128943	10.281033242
Ta4	3.065399212	2.561079205	11.950107871
Ta5	1.369920213	0.533022325	10.211698405
Ta6	6.512607417	0.595401176	11.919575601
Ta7	8.925142051	5.720422102	10.253232344
Ta8	3.764229736	5.782984017	11.956090810
Ta9	1.461082563	4.524406216	10.247690373
Ta10	6.518693311	4.542707748	11.946018895
Ta11	8.859991306	9.712546903	10.242125886
Ta12	3.759513067	9.732186158	11.908351582
Ta13	2.034891682	7.757359951	14.065027963
Ta14	7.210525349	7.791337744	15.906942807
Ta15	8.302769330	2.610360962	14.067895331
Ta16	3.118585619	2.574388323	15.868050565
Ta17	1.342042862	0.586542746	14.028875616
Ta18	6.486131273	0.598422563	15.821186236
Ta19	8.973251070	5.788533238	14.085773145
Ta20	3.749170925	5.853688606	15.944470602
Ta21	1.390244505	4.574987870	14.095676796
Ta22	6.469852820	4.588785988	15.877901947
Ta23	8.956529003	9.764186741	14.044644052
Ta24	3.767696324	9.728305607	15.833765807
Ta25	2.111975056	7.770986655	17.987368609
Ta26	7.263319693	8.098288422	19.804506020
Ta27	8.289790232	2.601357736	17.906551171
Ta28	2.992000725	2.319238484	19.713239463
Ta29	1.344804915	0.537939237	17.883177327
Ta30	6.612929916	0.727909093	19.667329557
Ta31	8.971393163	5.833281835	17.986463108
Ta32	3.410918253	5.846380694	19.873211819
Ta33	1.408538081	4.527915808	18.004751311
Ta34	6.883551592	4.553187309	19.782810074
Ta35	8.958583440	9.766099630	17.910470099
Ta36	3.622946679	9.672694961	19.713854494
N1	8.038465859	7.783324795	10.134712025
N2	2.631685255	7.761119983	12.098867280
N3	2.252335168	2.591417682	10.112417278
N4	7.700049380	2.596310809	12.112589692
N5	0.424430739	6.349784002	9.808253018
N6	3.053254979	5.971408616	10.097937385

N7	5.677850196	6.381372630	11.950182632
N8	8.440735027	5.910473545	12.103470480
N9	9.856287299	1.128202380	9.747458713
N10	7.224869175	0.818006584	10.097245819
N11	4.603041359	1.189514495	11.914928832
N12	1.864449773	0.722128626	12.059433874
N13	0.377349336	9.080754904	10.413324073
N14	2.959733627	9.521793545	9.976285548
N15	5.637689225	9.113749853	11.926011394
N16	8.344414056	9.661716970	12.100669723
N17	9.906263121	3.890569170	10.331400923
N18	7.293243203	4.340342511	10.022441704
N19	4.650090200	3.916689514	11.960195594
N20	1.919844689	4.447660712	12.104297472
N21	7.892661427	7.778272695	13.993533902
N22	2.754048355	7.789342227	15.965259403
N23	2.384626813	2.581003196	13.981354705
N24	7.587875152	2.607440859	15.981409840
N25	0.475835806	6.432087696	14.099247353
N26	3.165214690	5.916823466	13.981378887
N27	5.630139157	6.439845639	15.927060356
N28	8.377189917	5.978106439	16.027873763
N29	9.835489404	1.232824295	14.070698966
N30	7.116303524	0.788646892	13.954382934
N31	4.650798900	1.234202991	15.818381190
N32	1.962275856	0.702454684	15.957274301
N33	0.461443165	9.122456052	14.044779630
N34	3.184584755	9.627463659	13.907233854
N35	5.638496804	9.132111918	15.849378319
N36	8.345173464	9.631044865	15.973485655
N37	9.850299274	3.948716961	14.098533349
N38	7.108136962	4.435821539	13.969916129
N39	4.647943148	3.941032265	15.875680938
N40	1.946792391	4.417111662	16.040205056
N41	7.825246957	7.854546792	17.908371620
N42	2.874215402	7.822080425	20.009675383
N43	2.493839653	2.503524405	17.859659190
N44	7.484549977	2.568850590	19.880607501
N45	0.537101234	6.385513048	18.078847296
N46	3.254523050	5.887490214	17.945284579
N47	2.234034923	4.238276341	20.020508353
N48	8.140733901	6.051983446	19.920943940
N49	9.831499639	1.232062862	17.880419565
N50	7.033205935	0.759857371	17.831544424
N51	4.684460400	1.340689261	19.927895719
N52	1.987015317	0.664781875	19.905782877
N53	0.467161941	9.100706504	17.937284969
N54	3.268944537	9.650694433	17.844090931
N55	5.605484864	9.119017845	19.855905954

N56	8.273619135	9.732745716	19.933981309
N57	9.827623420	3.968499795	18.013362860
N58	7.068007085	4.465417148	17.876700918
N59	5.202227261	5.310702762	20.370937019
N60	6.917505456	7.484723570	22.041615037
H1	6.597443170	8.211244328	22.684959252
H2	6.178871596	6.768340416	21.956011465
H3	7.746006875	7.027157845	22.428883866

Structure O

Ta1	1.982420484	7.745018516	10.286430793
Ta2	7.234861065	7.754102022	11.976717000
Ta3	8.318001556	2.580408102	10.295463397
Ta4	3.084410403	2.564391224	11.970751044
Ta5	1.384707720	0.542654119	10.232619437
Ta6	6.527763126	0.588361787	11.936853934
Ta7	8.901611372	5.750361025	10.260038810
Ta8	3.783459067	5.776541960	11.951423624
Ta9	1.421297005	4.524844723	10.272149474
Ta10	6.539573618	4.540781566	11.970870849
Ta11	8.867744803	9.720735186	10.237105244
Ta12	3.780012256	9.723455754	11.923969855
Ta13	2.013545934	7.752706652	14.088933493
Ta14	7.213721765	7.784439562	15.906417880
Ta15	8.297521846	2.609049540	14.089991731
Ta16	3.127419362	2.579400800	15.876145562
Ta17	1.339295813	0.586005571	14.053259322
Ta18	6.540401943	0.615284242	15.853331849
Ta19	8.940663180	5.799474847	14.115799583
Ta20	3.815979070	5.782373139	15.913230059
Ta21	1.353122208	4.571681177	14.110864083
Ta22	6.553694218	4.564650162	15.936269329
Ta23	8.954211822	9.760760116	14.057946649
Ta24	3.818290988	9.771244827	15.829394440
Ta25	2.045805219	7.777521322	17.955802315
Ta26	7.334412908	8.077882584	19.748331781
Ta27	8.279131134	2.621705731	17.974441495
Ta28	3.051179641	2.344342667	19.713272781
Ta29	1.378081414	0.577694404	17.916003597
Ta30	6.682872155	0.726268981	19.724340599
Ta31	8.906248325	5.852111101	18.037275092
Ta32	3.428675343	5.839789909	19.852273689
Ta33	1.376575574	4.574299925	18.017697952
Ta34	6.922968276	4.545902607	19.873417138
Ta35	8.978559489	9.836607096	17.915651521
Ta36	3.715368015	9.694060436	19.697018700
N1	8.053098717	7.760142058	10.135233911
N2	2.588495872	7.753525034	12.121954520
N3	2.252955786	2.576514598	10.145235167

N4	7.694959571	2.578516872	12.126021243
N5	0.438710783	6.336712295	9.845644784
N6	3.089771060	5.987263607	10.109913760
N7	5.690846850	6.381355516	11.969953514
N8	8.441101385	5.895704160	12.111441694
N9	9.867369379	1.155804063	9.828428315
N10	7.226152603	0.798350525	10.097890743
N11	4.616190114	1.181495516	11.946380189
N12	1.874210929	0.689030464	12.086515629
N13	0.398281208	9.079412004	10.259079928
N14	3.021275866	9.513885211	10.027864736
N15	5.659544249	9.105355830	11.948892482
N16	8.382660115	9.658711016	12.096040813
N17	9.904549201	3.881039678	10.317058501
N18	7.294153577	4.344805746	10.043241698
N19	4.654669250	3.916420205	11.972644114
N20	1.923980817	4.469439013	12.130893889
N21	7.922944185	7.784396280	13.997669703
N22	2.726185911	7.780879828	16.011461483
N23	2.399711276	2.578179366	13.989591315
N24	7.587898735	2.599595886	15.999767238
N25	0.465708577	6.418294578	14.116523471
N26	3.205370024	5.957081664	14.012204697
N27	5.659460742	6.435462044	15.926862393
N28	8.363900817	5.951512003	16.052519976
N29	9.848422804	1.236362470	14.075516515
N30	7.131793270	0.764539467	13.964664852
N31	4.681170438	1.237199138	15.845920144
N32	1.988888340	0.722042543	15.977117552
N33	0.466684556	9.122417802	14.090617410
N34	3.203291660	9.576952077	13.944480961
N35	5.663599444	9.138114288	15.857865071
N36	8.357520257	9.660138555	15.987370318
N37	9.846995280	3.937327625	14.132754512
N38	7.126899175	4.429157649	13.985659619
N39	4.684573746	3.936730289	15.902113410
N40	1.955086005	4.410668463	16.047577367
N41	7.826666845	7.877278430	17.888114760
N42	2.864178129	7.840903735	19.916718049
N43	2.535673854	2.519796060	17.871827022
N44	7.508404258	2.568375819	19.967229833
N45	0.499840964	6.415670963	18.065284964
N46	3.258415035	5.922743496	17.936062810
N47	2.226520141	4.265004043	19.992968619
N48	8.082739304	6.150001800	20.040746449
N49	9.879233287	1.272774984	17.927771680
N50	7.078701604	0.754448368	17.867933142
N51	4.734599809	1.327293012	19.877146284
N52	2.060507332	0.687132047	19.921335538

N53	0.497697994	9.140464708	17.919288140
N54	3.309226737	9.624902364	17.855724858
N55	5.654822330	9.096564360	19.956731502
N56	8.349068539	9.723758066	19.922444188
N57	9.818761046	4.000308801	18.061594735
N58	7.075889480	4.464844663	17.947328781
N59	5.152119284	5.154550537	20.324827529