10.1071/CH09447_AC; CSIRO 2009.
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Accessory Publication

Microwave-Induced Molecular Rearrangements. Flash Thermolysis in the Gas-Phase and in Solution: Synthesis of Quinolones and Naphthyridones

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Contents:

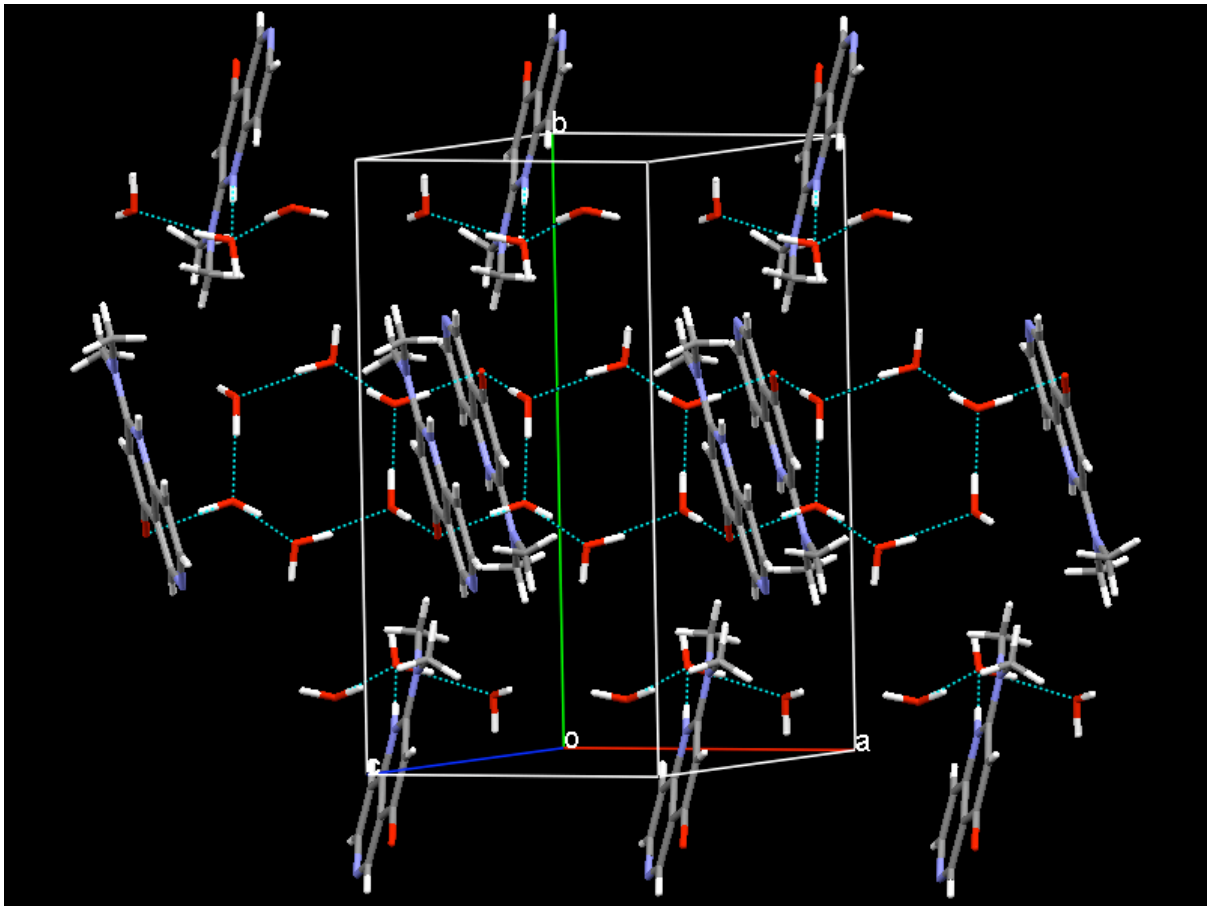


Fig. S1. Packing diagram for compound **11**·3H_2O. View generated with Mercury vers. 2.2 (Cambridge Crystallographic Data Centre, http://www.ccdc.cam.ac.uk/mercury/).

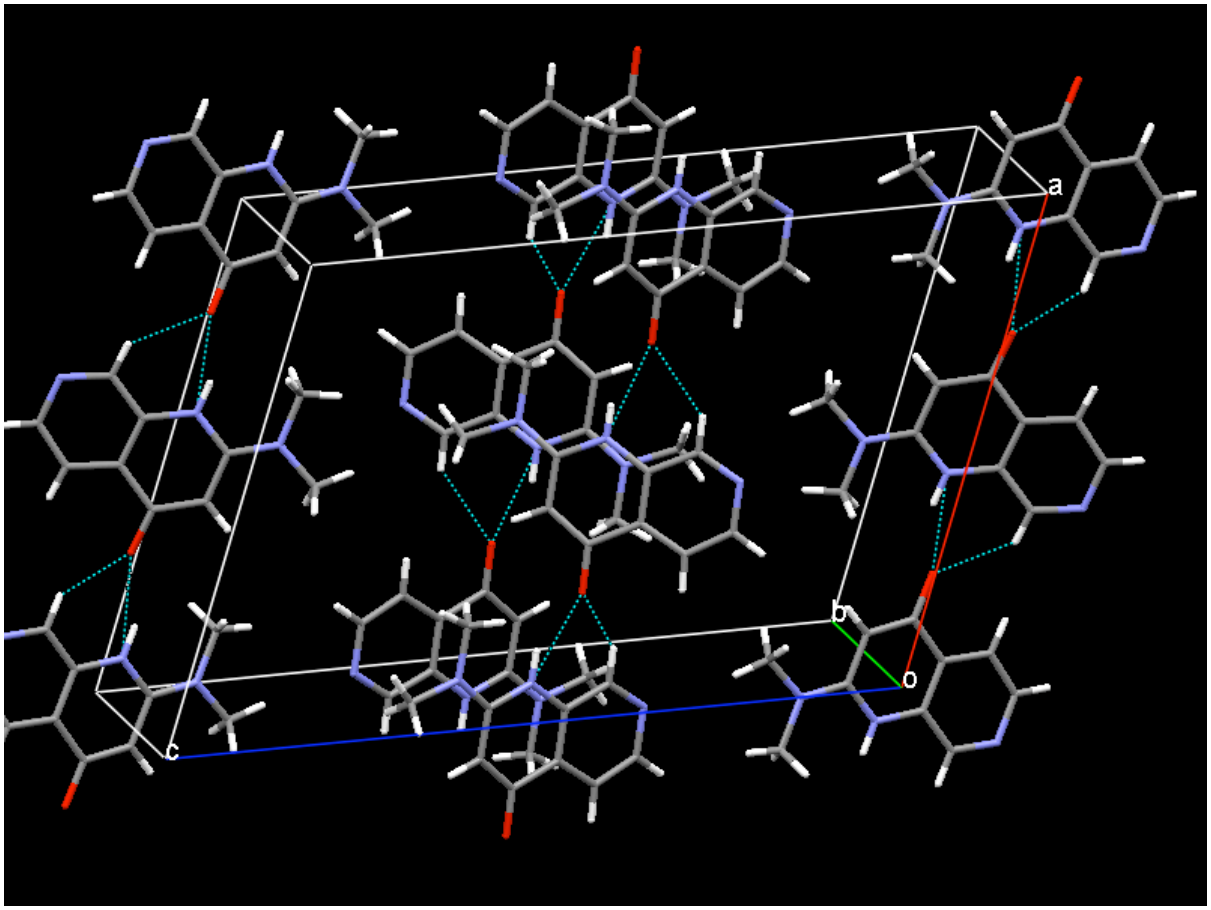


Fig. S2. Packing diagram for compound **16**. View generated with Mercury vers. 2.2 (Cambridge Crystallographic Data Centre, http://www.ccdc.cam.ac.uk/mercury/).

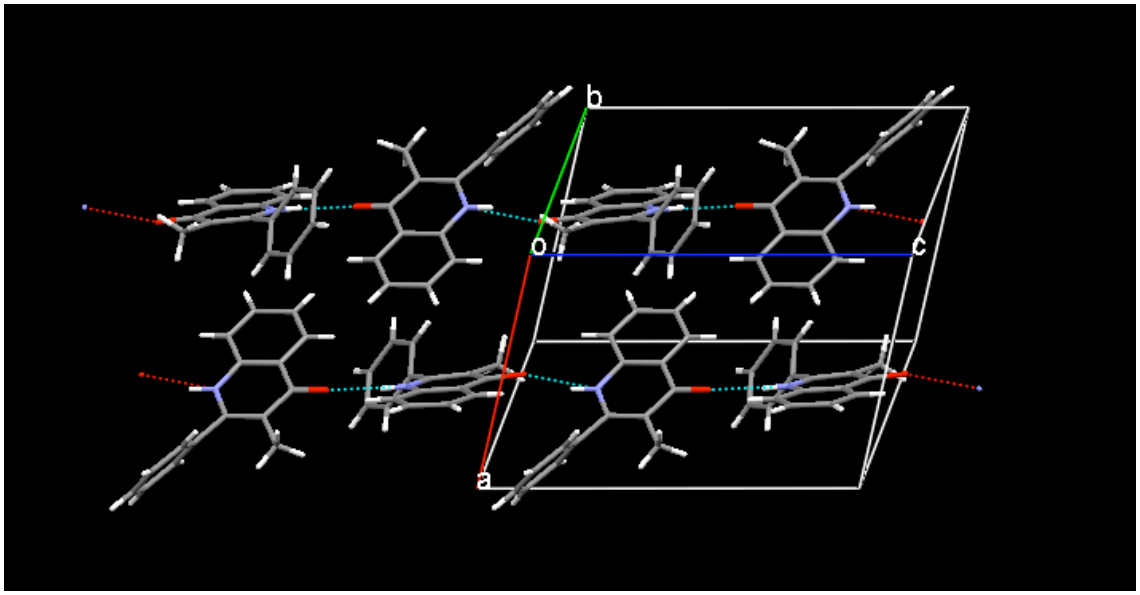
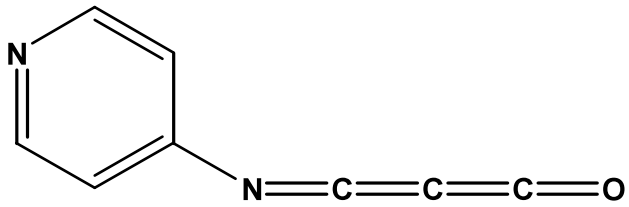


Fig. S3. Packing diagram for compound **24a**. View generated with Mercury vers. 2.2 (Cambridge Crystallographic Data Centre, http://www.ccdc.cam.ac.uk/mercury/).

Computational data

4-Pyridyliminopropadienone



Method: B3LYP/6-31G**. Calculations at other levels of theory (B3LYP/6-31G* and B3LYP/6-311++G*) have been reported previously.[i]

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	3.601906	0.539260	0.000039
2	6	3.280714	-0.760964	0.000054
3	6	1.974151	-1.244596	0.000006
4	6	0.925568	-0.317230	-0.000031
5	6	1.241200	1.050633	-0.000033
6	6	2.585369	1.412615	-0.000012
7	7	-0.382471	-0.769180	-0.000066
8	6	-1.537901	-0.409692	-0.000029
9	6	-2.794417	-0.149118	-0.000008
10	6	-4.042177	0.117109	0.000020
11	8	-5.190928	0.364759	0.000045
12	1	4.115377	-1.459542	0.000070
13	1	1.763954	-2.308606	0.000001
14	1	0.456980	1.800928	-0.000055
15	1	2.860027	2.466045	0.000004

Energy = -491.9141411

E+ZPVE = -491.811565

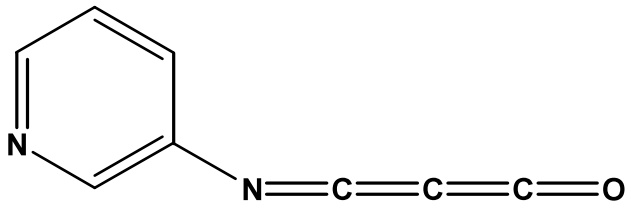
Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	41.2	1.4	0
2	A	42.3	0.4	0
3	A	130.3	0.2	0
4	A	137.9	3.3	0
5	A	238.7	3.9	0
6	A	333.1	7.5	0
7	A	378.5	0.0	0
8	A	416.7	13.8	0
9	A	507.4	8.5	0
10	A	511.8	9.4	0
11	A	533.6	37.4	1
12	A	547.3	60.6	1
13	A	557.0	50.8	1
14	A	650.5	7.4	0
15	A	680.0	17.8	0
16	A	715.3	1.0	0
17	A	805.8	37.4	1
18	A	835.8	1.3	0
19	A	880.6	2.2	0
20	A	937.4	0.5	0
21	A	955.8	0.0	0
22	A	971.5	5.0	0
23	A	1047.4	0.2	0
24	A	1071.1	0.7	0
25	A	1194.1	27.7	1
26	A	1218.9	4.1	0
27	A	1246.2	15.2	0

28	A	1313.1	1.1	0
29	A	1403.4	13.6	0
30	A	1472.9	27.1	1
31	A	1545.2	41.4	1
32	A	1573.2	255.4	5
33	A	1633.8	429.6	9
34	A	2158.0	134.8	3
35	A	2284.4	4721.0	100
36	A	3055.1	26.4	1
37	A	3059.4	26.6	1
38	A	3094.4	4.2	0
39	A	3104.2	4.3	0

3-Pyridyliminopropadienone



Method: B3LYP/6-31G**. Calculations at other levels of theory (B3LYP/6-31G* and B3LYP/6-311++G*) have been reported previously.[1]

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.565618	0.410597	-0.000184
2	7	3.260717	-0.893672	-0.000115
3	6	1.970927	-1.229214	0.000124
4	6	0.928950	-0.287520	0.000097
5	6	1.259326	1.076062	0.000113
6	6	2.604702	1.424729	0.000026
7	7	-0.379632	-0.736411	0.000077
8	6	-1.537873	-0.390068	0.000030

9	6	-2.797424	-0.137717	-0.000004
10	6	-4.046844	0.117120	-0.000045
11	8	-5.198474	0.355629	-0.000081
12	1	4.625118	0.656381	-0.000188
13	1	1.727823	-2.289341	-0.000092
14	1	0.475975	1.827503	0.000184
15	1	2.906987	2.467061	0.000068

Method: B3LYP/6-31G**
Energy = -491.9191363
E+ZPVE = -491.816758

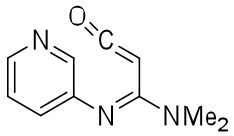
Vibrational Frequencies:

Scaled by a factor of 0.9613

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	42.4	3.2	0
2	A	43.0	0.7	0
3	A	130.3	0.0	0
4	A	137.3	5.0	0
5	A	239.9	0.2	0
6	A	327.9	9.0	0
7	A	399.6	2.0	0
8	A	423.6	5.4	0
9	A	486.3	0.3	0
10	A	501.1	10.9	0
11	A	529.6	33.1	1
12	A	551.1	39.8	1
13	A	558.9	59.9	1
14	A	599.7	4.5	0
15	A	689.8	19.1	0
16	A	699.9	5.6	0
17	A	786.8	24.9	1
18	A	870.1	12.4	0

19	A	898.4	0.7	0
20	A	924.6	2.5	0
21	A	954.2	0.1	0
22	A	995.0	14.9	0
23	A	1027.5	0.3	0
24	A	1099.9	9.0	0
25	A	1179.4	11.3	0
26	A	1206.8	35.3	1
27	A	1250.7	10.8	0
28	A	1310.1	1.7	0
29	A	1405.6	56.7	1
30	A	1454.0	23.6	0
31	A	1549.3	2.5	0
32	A	1570.8	8.2	0
33	A	1633.7	345.8	7
34	A	2157.9	92.0	2
35	A	2283.3	4738.1	100
36	A	3053.9	16.1	0
37	A	3059.9	8.5	0
38	A	3076.5	10.8	0
39	A	3090.2	7.4	0

N,N-Dimethylamino-3-pyridylimidoylketene 14



Method: B3LYP/6-31G*

Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.491960	-0.477874	-1.157816
C	0.846990	-0.724292	0.073885
C	1.667602	-0.846957	1.207114
C	3.568262	-0.425353	-0.197698
H	0.892500	-0.411826	-2.064785
H	1.213782	-1.063756	2.170072
H	4.639752	-0.296021	-0.338793

N	-0.528027	-0.941100	0.162832
C	-1.385063	-0.002891	-0.073889
N	-2.724052	-0.340629	-0.196113
C	-3.784973	0.523148	0.308945
H	-4.675681	0.422208	-0.321137
H	-4.062998	0.255076	1.340692
H	-3.477933	1.568488	0.309861
C	-3.055319	-1.760045	-0.154876
H	-3.024574	-2.163926	0.867841
H	-4.065015	-1.890862	-0.557579
H	-2.342620	-2.320985	-0.759265
C	-1.078390	1.428728	-0.286724
H	-1.788843	2.064217	-0.804695
C	0.049554	2.044995	0.045134
O	0.987743	2.681128	0.318736
N	2.809970	-0.328250	-1.297785
C	3.043182	-0.688141	1.068648
H	3.701613	-0.769693	1.929023

Method: RB3LYP/6-31G(d), HF= -627.11476892 Hartree
RMSD=7.838e-09 and RMSF=9.682e-06
Zero-point correction= 0.198259 (Hartree/Particle)
Sum of electronic and zero-point Energies= -626.916510 Hartree

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	31,0	1,0	0
2	A	50,0	1,0	0
3	A	64,0	0,0	0
4	A	75,0	0,0	0
5	A	109,0	0,0	0
6	A	110,0	4,0	0
7	A	152,0	0,0	0
8	A	166,0	0,0	0
9	A	232,0	1,0	0
10	A	237,0	12,0	1
11	A	277,0	5,0	0
12	A	348,0	1,0	0
13	A	403,0	2,0	0
14	A	423,0	7,0	1
15	A	429,0	1,0	0
16	A	452,0	2,0	0
17	A	484,0	5,0	0
18	A	515,0	0,0	0
19	A	526,0	27,0	4
20	A	570,0	5,0	0
21	A	604,0	9,0	1
22	A	641,0	3,0	0
23	A	694,0	21,0	3
24	A	700,0	18,0	2
25	A	783,0	18,0	2
26	A	812,0	13,0	1
27	A	863,0	2,0	0
28	A	891,0	0,0	0
29	A	914,0	1,0	0
30	A	945,0	11,0	1
31	A	947,0	8,0	1
32	A	993,0	7,0	1
33	A	1029,0	0,0	0

34	A	1045,0	14,0	2
35	A	1088,0	17,0	2
36	A	1093,0	26,0	3
37	A	1098,0	72,0	10
38	A	1116,0	136,0	20
39	A	1134,0	20,0	3
40	A	1180,0	7,0	1
41	A	1203,0	26,0	3
42	A	1245,0	6,0	0
43	A	1263,0	91,0	13
44	A	1313,0	3,0	0
45	A	1336,0	33,0	5
46	A	1395,0	236,0	35
47	A	1399,0	18,0	2
48	A	1411,0	8,0	1
49	A	1440,0	31,0	4
50	A	1448,0	1,0	0
51	A	1458,0	9,0	1
52	A	1462,0	29,0	4
53	A	1472,0	9,0	1
54	A	1497,0	30,0	4
55	A	1547,0	5,0	0
56	A	1570,0	74,0	11
57	A	1605,0	573,0	87
58	A	2132,0	657,0	100
59	A	2890,0	70,0	10
60	A	2909,0	68,0	10
61	A	2969,0	36,0	5
62	A	2981,0	42,0	6
63	A	3047,0	25,0	3
64	A	3052,0	12,0	1
65	A	3053,0	16,0	2
66	A	3053,0	9,0	1
67	A	3072,0	21,0	3
68	A	3087,0	19,0	2
69	A	3090,0	8,0	1

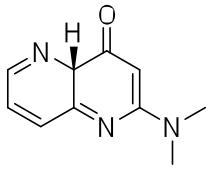
TS connecting 14 and 17

Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	-1.343023	0.360669	0.682894
C	-0.798013	-0.843860	0.114795
C	-1.732706	-1.786170	-0.417828
C	-3.497178	-0.219032	0.122419
H	-0.820173	0.774039	1.549362
H	-1.352250	-2.719197	-0.822784
H	-4.556539	0.035623	0.101910
N	0.514247	-1.082233	0.026792
C	1.362813	-0.044502	-0.029071
N	2.694175	-0.334246	0.070771
C	3.718486	0.696985	0.062438
H	4.576083	0.343570	0.643681
H	4.069561	0.932880	-0.952877
H	3.341698	1.611045	0.526768
C	3.176344	-1.708716	0.106816
H	3.901867	-1.873608	-0.700542
H	3.671599	-1.917393	1.064141
H	2.331750	-2.383398	-0.015888

C	0.976864	1.305048	-0.312678
H	1.665369	1.955225	-0.842109
C	-0.314204	1.794391	-0.235528
O	-0.944796	2.789278	-0.402845
N	-2.692157	0.638647	0.690458
C	-3.063599	-1.467887	-0.427420
H	-3.799154	-2.149730	-0.846063

RB3LYP/6-31G(d), HF= -627.09545202
Zero-point correction=0.198359 (Hartree/Particle)
Sum of electronic and zero-point Energies= -626.897093
Negative frequency= -420.908 cm^{-1}

2-(Dimethylamino)-1,5-naphthyridin-4(4a*H*)-one 17



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.776214	-0.815882	0.110211
C	-1.724767	-1.893907	-0.067129
C	-3.494076	-0.217632	-0.056784
H	-1.332240	-2.899720	-0.185095
H	-4.555500	-0.015012	-0.214232
N	0.493789	-1.066619	0.009585
C	1.387531	0.004265	0.013383
N	2.705592	-0.360398	0.090308
C	3.736274	0.661948	0.119762
H	4.668236	0.211785	0.471969
H	3.918370	1.104609	-0.871284
H	3.454756	1.463223	0.809615
C	3.161354	-1.723708	-0.153281
H	3.666229	-1.800718	-1.127445
H	3.872420	-2.021304	0.626568
H	2.307259	-2.396181	-0.140354
C	0.982387	1.325617	-0.106737
H	1.681179	2.113511	-0.358277
C	-0.408448	1.699541	-0.077312
O	-0.848343	2.811067	-0.324688
C	-1.338303	0.548861	0.428472
H	-1.204263	0.666382	1.523409
C	-3.044408	-1.604431	-0.149844
N	-2.741367	0.792646	0.188342
H	-3.783783	-2.382547	-0.319451

RB3LYP/6-31G(d), HF=-627.109141448 Hartree
RMSD=3.192e-09 and RMSF=3.681e-06
Zero-point correction= 0.200253 (Hartree/Particle)
Sum of electronic and zero-point Energies= -626.909161 Hartree

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.

1	A	54,0	1,0	0
2	A	69,0	1,0	0
3	A	98,0	3,0	0
4	A	143,0	1,0	0
5	A	150,0	1,0	0
6	A	164,0	0,0	0
7	A	208,0	5,0	1
8	A	231,0	3,0	0
9	A	264,0	0,0	0
10	A	301,0	0,0	0
11	A	332,0	1,0	0
12	A	382,0	4,0	0
13	A	399,0	5,0	1
14	A	447,0	5,0	1
15	A	487,0	1,0	0
16	A	491,0	4,0	0
17	A	529,0	5,0	1
18	A	580,0	9,0	1
19	A	588,0	2,0	0
20	A	605,0	12,0	2
21	A	660,0	4,0	0
22	A	682,0	11,0	2
23	A	757,0	45,0	9
24	A	771,0	8,0	1
25	A	821,0	14,0	2
26	A	849,0	5,0	1
27	A	867,0	20,0	4
28	A	935,0	0,0	0
29	A	947,0	1,0	0
30	A	968,0	32,0	6
31	A	976,0	1,0	0
32	A	992,0	25,0	5
33	A	1046,0	10,0	2
34	A	1051,0	24,0	5
35	A	1085,0	19,0	4
36	A	1092,0	5,0	1
37	A	1122,0	18,0	3
38	A	1130,0	59,0	12
39	A	1146,0	53,0	11
40	A	1184,0	90,0	19
41	A	1211,0	3,0	0
42	A	1220,0	0,0	0
43	A	1268,0	2,0	0
44	A	1325,0	27,0	5
45	A	1357,0	8,0	1
46	A	1374,0	168,0	35
47	A	1398,0	1,0	0
48	A	1407,0	9,0	1
49	A	1429,0	24,0	5
50	A	1457,0	13,0	2
51	A	1467,0	26,0	5
52	A	1475,0	39,0	8
53	A	1481,0	8,0	1
54	A	1534,0	132,0	28
55	A	1554,0	41,0	8
56	A	1584,0	469,0	99
57	A	1643,0	0,0	0
58	A	1706,0	382,0	81
59	A	2820,0	2,0	0
60	A	2899,0	29,0	6
61	A	2907,0	120,0	25

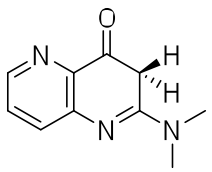
62	A	2963,0	43,0	9
63	A	2980,0	24,0	5
64	A	3018,0	52,0	11
65	A	3020,0	14,0	2
66	A	3074,0	6,0	1
67	A	3085,0	1,0	0
68	A	3093,0	12,0	2
69	A	3112,0	6,0	1

TS connecting 17 and 19

Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	-0.814708	-0.777722	-0.162554
C	-1.769019	-1.837446	-0.230318
C	-3.490050	-0.228980	0.308891
H	-1.408277	-2.834174	-0.465985
H	-4.541524	-0.020077	0.505939
N	0.489947	-1.049547	-0.293332
C	1.356283	-0.057597	-0.025706
N	2.693189	-0.365787	-0.022185
C	3.704138	0.642313	0.247526
H	4.678183	0.242774	-0.046023
H	3.523064	1.547842	-0.339823
H	3.756626	0.919752	1.311392
C	3.147196	-1.751363	-0.033681
H	3.930321	-1.880624	-0.790078
H	3.559051	-2.039969	0.944496
H	2.305863	-2.398086	-0.272297
C	0.902759	1.267391	0.291273
H	1.617495	2.049641	0.525631
C	-0.418938	1.710566	-0.219903
O	-0.736662	2.824213	-0.569168
C	-1.335948	0.550028	0.134679
H	-0.391701	0.823518	1.170294
N	-2.676589	0.795046	0.332251
C	-3.088912	-1.568585	0.010060
H	-3.838434	-2.353908	-0.028935

RB3LYP/6-31G(d), HF= -627. 06170716
Zero-point correction= 0.195111 (Hartree/Particle)
Sum of electronic and zero-point Energies= - -626.866596
Negative frequency= -1612.97 cm^{-1}

2-(Dimethylamino)-1,5-naphthyridin-4(3*H*)-one 19



Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	0.841170	-0.765628	-0.000010
C	1.736452	-1.854193	0.017686

C	3.555039	-0.284121	0.025811
H	1.327321	-2.859953	0.020427
H	4.621840	-0.066747	0.035875
N	-0.518443	-1.047886	-0.007682
C	-1.379741	-0.072172	-0.036688
N	-2.712183	-0.378932	-0.110875
C	-3.760708	0.599545	0.137013
H	-4.668015	0.285082	-0.387212
H	-4.001399	0.689792	1.207831
H	-3.484969	1.584915	-0.239342
C	-3.123414	-1.778207	-0.049222
H	-3.257085	-2.115688	0.988655
H	-4.072623	-1.892165	-0.581532
H	-2.357363	-2.396664	-0.513460
C	-0.996358	1.394201	-0.014788
H	-1.412377	1.883968	0.875576
C	0.507908	1.702346	-0.022816
O	0.875972	2.862446	-0.040118
C	1.413799	0.530383	-0.003253
H	-1.432744	1.922826	-0.871318
N	2.738847	0.762638	0.009318
C	3.099334	-1.613965	0.030619
H	3.811211	-2.434806	0.044006

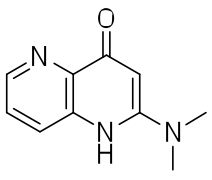
RB3LYP/6-31G(d), HF=-627.15843728 Hartree
RMSD=2.422e-09 and RMSF=6.319e-06
Zero-point correction= 0.200919 (Hartree/Particle)
Sum of electronic and zero-point Energies= -626.957518Hartree

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	26,0	5,0	0
2	A	67,0	0,0	0
3	A	71,0	1,0	0
4	A	102,0	0,0	0
5	A	116,0	0,0	0
6	A	145,0	6,0	0
7	A	193,0	1,0	0
8	A	206,0	11,0	1
9	A	289,0	1,0	0
10	A	295,0	2,0	0
11	A	334,0	0,0	0
12	A	382,0	4,0	0
13	A	410,0	3,0	0
14	A	463,0	0,0	0
15	A	481,0	3,0	0
16	A	492,0	0,0	0
17	A	519,0	4,0	0
18	A	540,0	1,0	0
19	A	610,0	15,0	2
20	A	615,0	5,0	0
21	A	625,0	4,0	0
22	A	714,0	6,0	0
23	A	746,0	9,0	1
24	A	801,0	24,0	3
25	A	843,0	17,0	2
26	A	851,0	1,0	0
27	A	909,0	1,0	0
28	A	920,0	5,0	0

29	A	952,0	46,0	7
30	A	959,0	0,0	0
31	A	1022,0	0,0	0
32	A	1047,0	8,0	1
33	A	1059,0	3,0	0
34	A	1088,0	5,0	0
35	A	1093,0	15,0	2
36	A	1121,0	169,0	26
37	A	1140,0	8,0	1
38	A	1171,0	28,0	4
39	A	1180,0	1,0	0
40	A	1205,0	25,0	3
41	A	1259,0	93,0	14
42	A	1273,0	4,0	0
43	A	1294,0	48,0	7
44	A	1298,0	7,0	1
45	A	1390,0	92,0	14
46	A	1397,0	159,0	24
47	A	1400,0	7,0	1
48	A	1409,0	119,0	18
49	A	1439,0	9,0	1
50	A	1450,0	11,0	1
51	A	1460,0	14,0	2
52	A	1465,0	19,0	2
53	A	1474,0	17,0	2
54	A	1502,0	7,0	1
55	A	1535,0	29,0	4
56	A	1566,0	640,0	100
57	A	1589,0	273,0	42
58	A	1724,0	235,0	36
59	A	2896,0	68,0	10
60	A	2915,0	78,0	12
61	A	2933,0	2,0	0
62	A	2968,0	2,0	0
63	A	2986,0	1,0	0
64	A	2989,0	66,0	10
65	A	3047,0	12,0	1
66	A	3049,0	19,0	2
67	A	3070,0	1,0	0
68	A	3076,0	24,0	3
69	A	3093,0	14,0	2

2-(Dimethylamino)-1,5-naphthyridin-4(1*H*)-one



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.910890	-0.774387	-0.082500
C	1.846404	-1.818615	-0.155960
C	3.563140	-0.153174	0.025170
H	1.511891	-2.849871	-0.248588
H	4.615165	0.123472	0.071846
N	-0.450357	-1.037013	-0.126976

C	-1.397802	-0.028054	-0.090599
N	-2.714970	-0.477017	-0.228232
C	-3.725932	0.533356	-0.511615
H	-4.641661	0.026088	-0.831076
H	-3.966777	1.158823	0.363679
H	-3.384861	1.180498	-1.322481
C	-3.187446	-1.495202	0.716057
H	-3.499349	-1.050090	1.675012
H	-4.044269	-2.020308	0.282126
H	-2.405036	-2.226568	0.926095
C	-1.006180	1.275341	0.036002
H	-1.740786	2.064268	0.131565
C	0.391091	1.684526	0.093987
O	0.739731	2.856682	0.206652
C	1.376417	0.554049	0.036603
H	-0.747083	-1.935283	-0.483964
C	3.192651	-1.501868	-0.104560
N	2.687578	0.842336	0.093352
H	3.949755	-2.278456	-0.159950

RB3LYP/6-31G(d), HF=-627.15617028 Hartree
RMSD=3.893e-09 and RMSF=2.198e-05
Zero-point correction= 0.202044 (Hartree/Particle)
Sum of electronic and zero-point Energies= -626.954126Hartree

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	55,0	2,0	0
2	A	71,0	1,0	0
3	A	118,0	0,0	0
4	A	150,0	1,0	0
5	A	164,0	2,0	0
6	A	183,0	0,0	0
7	A	240,0	5,0	1
8	A	264,0	1,0	0
9	A	287,0	4,0	1
10	A	312,0	3,0	0
11	A	328,0	7,0	1
12	A	379,0	8,0	2
13	A	430,0	4,0	1
14	A	451,0	23,0	6
15	A	466,0	56,0	15
16	A	489,0	29,0	8
17	A	520,0	0,0	0
18	A	529,0	1,0	0
19	A	604,0	6,0	1
20	A	623,0	3,0	0
21	A	657,0	3,0	0
22	A	673,0	2,0	0
23	A	729,0	3,0	0
24	A	767,0	12,0	3
25	A	780,0	34,0	9
26	A	817,0	26,0	7
27	A	846,0	10,0	2
28	A	896,0	17,0	4
29	A	899,0	8,0	2
30	A	942,0	0,0	0
31	A	987,0	39,0	11
32	A	1038,0	5,0	1

33	A	1045,0	12,0	3
34	A	1086,0	16,0	4
35	A	1090,0	7,0	1
36	A	1113,0	7,0	1
37	A	1125,0	75,0	21
38	A	1138,0	12,0	3
39	A	1189,0	10,0	2
40	A	1199,0	51,0	14
41	A	1234,0	20,0	5
42	A	1281,0	27,0	7
43	A	1289,0	18,0	5
44	A	1308,0	4,0	1
45	A	1348,0	64,0	18
46	A	1406,0	167,0	47
47	A	1414,0	20,0	5
48	A	1436,0	5,0	1
49	A	1447,0	1,0	0
50	A	1452,0	11,0	3
51	A	1466,0	33,0	9
52	A	1474,0	13,0	3
53	A	1487,0	82,0	23
54	A	1493,0	83,0	23
55	A	1563,0	50,0	14
56	A	1579,0	86,0	24
57	A	1607,0	249,0	70
58	A	1680,0	354,0	100
59	A	2882,0	29,0	8
60	A	2887,0	107,0	30
61	A	2980,0	14,0	3
62	A	2981,0	50,0	14
63	A	3033,0	11,0	3
64	A	3035,0	23,0	6
65	A	3050,0	16,0	4
66	A	3055,0	20,0	5
67	A	3088,0	21,0	5
68	A	3122,0	2,0	0
69	A	3467,0	30,0	8

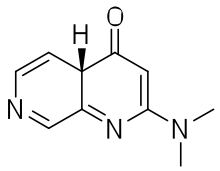
TS connecting 14 and 18

Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	-2.766415	0.580875	0.598979
C	-1.348374	0.396907	0.680324
C	-0.803452	-0.814141	0.142591
C	-1.740328	-1.767575	-0.386261
C	-3.539324	-0.383841	0.012006
H	-3.214345	1.489132	0.991178
H	-0.842491	0.828738	1.546535
H	-1.345473	-2.711765	-0.760041
H	-4.614720	-0.263455	-0.088726
N	-3.033433	-1.568729	-0.457029
N	0.506266	-1.069493	0.055222
C	1.364504	-0.044540	-0.021304
N	2.693732	-0.344104	0.067802
C	3.728989	0.676113	0.035738
H	4.590681	0.317853	0.607567
H	4.067805	0.899112	-0.986489
H	3.370329	1.598540	0.498052

C	3.162320	-1.723699	0.116259
H	3.883181	-1.902450	-0.691933
H	3.658496	-1.927327	1.074054
H	2.311078	-2.391541	0.002729
C	0.988625	1.309858	-0.312825
H	1.682698	1.949239	-0.848077
C	-0.287238	1.824490	-0.223957
O	-0.908631	2.832940	-0.357013

RB3LYP/6-31G(d), HF= -627. 09421779
Zero-point correction= 0.198173 (Hartree/Particle)
Sum of electronic and zero-point Energies= -626.896045
Negative frequency= -431.373 cm^{-1}

2-(Dimethylamino)-1,7-naphthyridin-4(4a*H*)-one 18



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.772300	0.710678	0.081169
C	-0.776765	-0.792282	0.151595
C	-1.745220	-1.875204	0.002202
C	-3.515864	-0.384186	-0.163918
H	-3.187232	1.712932	0.057754
H	-1.352939	-2.892091	-0.032554
H	-4.574086	-0.313024	-0.398086
N	-3.017386	-1.695100	-0.146411
N	0.487259	-1.056118	0.041664
C	1.388330	0.010710	0.015308
N	2.702791	-0.361326	0.060151
C	3.742704	0.653168	0.060217
H	4.682010	0.193291	0.377402
H	3.892883	1.098302	-0.934558
H	3.492950	1.453504	0.763501
C	3.144662	-1.735536	-0.151907
H	3.652070	-1.835230	-1.121960
H	3.849376	-2.024102	0.636921
H	2.283998	-2.399016	-0.128777
C	0.989304	1.338151	-0.098759
H	1.691704	2.122292	-0.351219
C	-0.393820	1.716059	-0.033024
O	-0.846246	2.838918	-0.232260
C	-1.330037	0.571454	0.431482
H	-1.255378	0.681543	1.535630

RB3LYP/6-31G(d), HF= -627.11119027 Hartree
RMSD=3.651e-09\RMSF=2.362e-05
Zero-point correction= 0.200132 (Hartree/Particle)
Sum of electronic and zero-point Energies= -626.911058Hartree

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	57,0	2,0	0
2	A	69,0	1,0	0
3	A	107,0	2,0	0
4	A	144,0	1,0	0
5	A	151,0	0,0	0
6	A	163,0	0,0	0
7	A	205,0	8,0	1
8	A	226,0	2,0	0
9	A	262,0	3,0	0
10	A	293,0	0,0	0
11	A	335,0	1,0	0
12	A	389,0	4,0	0
13	A	405,0	1,0	0
14	A	445,0	18,0	4
15	A	471,0	7,0	1
16	A	492,0	8,0	1
17	A	539,0	3,0	0
18	A	579,0	21,0	5
19	A	599,0	6,0	1
20	A	626,0	4,0	0
21	A	673,0	1,0	0
22	A	683,0	12,0	2
23	A	756,0	14,0	3
24	A	766,0	38,0	9
25	A	811,0	4,0	0
26	A	838,0	1,0	0
27	A	868,0	13,0	3
28	A	907,0	3,0	0
29	A	943,0	5,0	1
30	A	953,0	4,0	0
31	A	962,0	27,0	6
32	A	1006,0	3,0	0
33	A	1048,0	38,0	9
34	A	1054,0	0,0	0
35	A	1079,0	42,0	10
36	A	1092,0	5,0	1
37	A	1130,0	66,0	16
38	A	1140,0	42,0	10
39	A	1166,0	32,0	7
40	A	1196,0	37,0	9
41	A	1208,0	22,0	5
42	A	1217,0	7,0	1
43	A	1285,0	9,0	2
44	A	1323,0	8,0	1
45	A	1335,0	21,0	5
46	A	1369,0	48,0	11
47	A	1377,0	116,0	28
48	A	1405,0	2,0	0
49	A	1428,0	30,0	7
50	A	1458,0	13,0	3
51	A	1466,0	26,0	6
52	A	1474,0	32,0	7
53	A	1480,0	2,0	0
54	A	1515,0	13,0	3
55	A	1548,0	249,0	61
56	A	1592,0	385,0	94
57	A	1617,0	3,0	0
58	A	1686,0	407,0	99
59	A	2792,0	2,0	0
60	A	2904,0	28,0	6

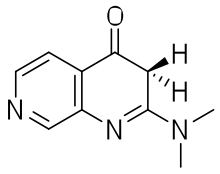
61	A	2912,0	109,0	26
62	A	2966,0	39,0	9
63	A	2981,0	21,0	5
64	A	3023,0	16,0	3
65	A	3040,0	16,0	3
66	A	3080,0	21,0	5
67	A	3087,0	1,0	0
68	A	3106,0	13,0	3
69	A	3115,0	4,0	0

TS connecting 18 and 20

Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	-2.741328	0.718671	0.260296
C	-0.811795	-0.764072	-0.140486
C	-1.776698	-1.826623	-0.174373
C	-3.534935	-0.394693	0.236496
H	-3.154287	1.715986	0.376014
H	-1.408512	-2.833466	-0.368459
H	-4.610888	-0.319367	0.371946
N	-3.062562	-1.664060	0.011884
N	0.489710	-1.047596	-0.267453
C	1.361724	-0.054790	-0.023877
N	2.696866	-0.364813	-0.029198
C	3.713521	0.644978	0.212821
H	4.683189	0.236778	-0.082636
H	3.530329	1.540693	-0.389035
H	3.777051	0.940615	1.271025
C	3.148746	-1.751829	-0.038940
H	3.916936	-1.887570	-0.809209
H	3.578403	-2.032154	0.933571
H	2.302592	-2.399686	-0.256277
C	0.917203	1.278512	0.282019
H	1.636871	2.057079	0.511684
C	-0.406945	1.725648	-0.198954
O	-0.748534	2.854361	-0.489120
C	-1.325747	0.565154	0.115505
H	-0.393992	0.835752	1.164674

RB3LYP/6-31G(d), HF= -627.06328592
Zero-point correction=0.195137 (Hartree/Particle)
Sum of electronic and zero-point Energies= -626.868149
Negative frequency= -1590.34 cm^{-1}

2-(Dimethylamino)-1,7-naphthyridin-4(3*H*)-one 20



Atom	Coordinates (Angstroms)		
Type	X	Y	Z

C	2.790098	0.691469	0.010194
C	0.839682	-0.751595	-0.001264
C	1.750577	-1.832418	0.015199
C	3.581213	-0.448404	0.025358
H	3.219617	1.688393	0.008786
H	1.349525	-2.844434	0.017541
H	4.666465	-0.374698	0.036156
N	3.071824	-1.696619	0.027773
N	-0.515817	-1.042160	-0.007388
C	-1.380574	-0.069533	-0.039232
N	-2.712742	-0.377807	-0.109318
C	-3.761746	0.602682	0.128154
H	-4.673808	0.271337	-0.376648
H	-3.989877	0.718748	1.199253
H	-3.496004	1.579784	-0.276792
C	-3.122749	-1.777367	-0.035664
H	-3.272462	-2.100119	1.004583
H	-4.063018	-1.900460	-0.581616
H	-2.347957	-2.400091	-0.479007
C	-1.003653	1.402296	-0.027346
H	-1.433564	1.902595	0.850168
C	0.497260	1.707683	-0.019677
O	0.880409	2.867522	-0.024303
C	1.397281	0.544596	-0.003786
H	-1.429378	1.918429	-0.897094

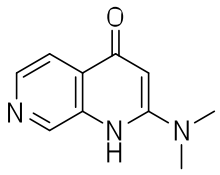
RB3LYP/6-31G(d), HF= -627.16247733 Hartree
RMSD=3.246e-09\RMSF=1.549e-06
Zero-point correction= 0.201125 (Hartree/Particle)
Sum of electronic and zero-point Energies= -626.961352Hartree

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	33,0	2,0	0
2	A	66,0	0,0	0
3	A	76,0	4,0	0
4	A	106,0	1,0	0
5	A	118,0	4,0	0
6	A	148,0	0,0	0
7	A	190,0	1,0	0
8	A	203,0	13,0	1
9	A	281,0	1,0	0
10	A	287,0	3,0	0
11	A	336,0	1,0	0
12	A	380,0	4,0	0
13	A	410,0	0,0	0
14	A	463,0	2,0	0
15	A	478,0	8,0	1
16	A	491,0	1,0	0
17	A	524,0	0,0	0
18	A	546,0	4,0	0
19	A	600,0	18,0	2
20	A	621,0	4,0	0
21	A	656,0	8,0	1
22	A	721,0	0,0	0
23	A	739,0	1,0	0
24	A	821,0	24,0	3
25	A	837,0	6,0	0
26	A	851,0	9,0	1

27	A	913,0	0,0	0
28	A	922,0	6,0	0
29	A	945,0	0,0	0
30	A	949,0	48,0	6
31	A	1030,0	5,0	0
32	A	1034,0	4,0	0
33	A	1048,0	10,0	1
34	A	1087,0	6,0	0
35	A	1116,0	213,0	27
36	A	1137,0	4,0	0
37	A	1159,0	4,0	0
38	A	1178,0	1,0	0
39	A	1197,0	29,0	3
40	A	1212,0	35,0	4
41	A	1251,0	96,0	12
42	A	1271,0	4,0	0
43	A	1284,0	55,0	7
44	A	1304,0	20,0	2
45	A	1385,0	227,0	29
46	A	1390,0	35,0	4
47	A	1401,0	5,0	0
48	A	1421,0	36,0	4
49	A	1441,0	25,0	3
50	A	1454,0	82,0	10
51	A	1461,0	3,0	0
52	A	1465,0	15,0	1
53	A	1473,0	18,0	2
54	A	1500,0	5,0	0
55	A	1530,0	76,0	9
56	A	1575,0	764,0	100
57	A	1582,0	105,0	13
58	A	1709,0	232,0	30
59	A	2896,0	68,0	8
60	A	2916,0	77,0	10
61	A	2934,0	1,0	0
62	A	2969,0	1,0	0
63	A	2988,0	3,0	0
64	A	2990,0	62,0	8
65	A	3044,0	12,0	1
66	A	3058,0	28,0	3
67	A	3062,0	14,0	1
68	A	3072,0	1,0	0
69	A	3096,0	10,0	1

2-(Dimethylamino)-1,7-naphthyridin-4(1*H*)-one 16



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.741298	0.772128	0.085377
C	0.907019	-0.762575	-0.078337
C	1.856362	-1.799357	-0.147089
C	3.596902	-0.317742	0.012242
H	3.106382	1.790000	0.175382

H	1.525437	-2.835430	-0.239930
H	4.675658	-0.184290	0.047569
N	3.165433	-1.589772	-0.106992
N	-0.454150	-1.028357	-0.124068
C	-1.399071	-0.020587	-0.086362
N	-2.716777	-0.457518	-0.219808
C	-3.730555	0.556261	-0.479330
H	-4.646250	0.052935	-0.804459
H	-3.968382	1.163465	0.409227
H	-3.395739	1.219243	-1.279866
C	-3.191956	-1.516456	0.676675
H	-3.529635	-1.108918	1.643194
H	-4.031939	-2.038475	0.207606
H	-2.404304	-2.243801	0.879366
C	-1.007266	1.289266	0.036793
H	-1.743409	2.076446	0.131695
C	0.385801	1.688635	0.089379
O	0.761853	2.858683	0.198004
C	1.358854	0.561039	0.034499
H	-0.748513	-1.934780	-0.460828

RB3LYP/6-31G(d), HF= -627.16384139 Hartree
RMSD=9.798e-09\RMSF=2.339e-06
Zero-point correction= 0.202461 (Hartree/Particle)
Sum of electronic and zero-point Energies=-626.961381Hartree

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	58,0	2,0	0
2	A	74,0	2,0	0
3	A	129,0	1,0	0
4	A	146,0	2,0	0
5	A	169,0	1,0	0
6	A	179,0	0,0	0
7	A	235,0	7,0	1
8	A	258,0	1,0	0
9	A	281,0	10,0	2
10	A	307,0	5,0	1
11	A	326,0	5,0	1
12	A	378,0	10,0	2
13	A	430,0	2,0	0
14	A	454,0	25,0	6
15	A	472,0	68,0	17
16	A	489,0	25,0	6
17	A	527,0	2,0	0
18	A	533,0	3,0	0
19	A	594,0	12,0	3
20	A	656,0	1,0	0
21	A	664,0	4,0	1
22	A	676,0	2,0	0
23	A	737,0	0,0	0
24	A	758,0	0,0	0
25	A	809,0	58,0	14
26	A	832,0	6,0	1
27	A	841,0	1,0	0
28	A	887,0	0,0	0
29	A	901,0	22,0	5
30	A	954,0	0,0	0
31	A	986,0	46,0	11

32	A	1033,0	10,0	2
33	A	1046,0	12,0	3
34	A	1086,0	3,0	0
35	A	1088,0	24,0	6
36	A	1121,0	94,0	23
37	A	1138,0	7,0	1
38	A	1169,0	10,0	2
39	A	1191,0	8,0	2
40	A	1225,0	9,0	2
41	A	1234,0	27,0	6
42	A	1278,0	50,0	12
43	A	1297,0	17,0	4
44	A	1317,0	9,0	2
45	A	1351,0	64,0	16
46	A	1397,0	42,0	10
47	A	1415,0	2,0	0
48	A	1446,0	5,0	1
49	A	1451,0	60,0	15
50	A	1455,0	78,0	19
51	A	1465,0	38,0	9
52	A	1474,0	12,0	3
53	A	1487,0	61,0	15
54	A	1494,0	113,0	28
55	A	1559,0	88,0	22
56	A	1580,0	122,0	30
57	A	1599,0	195,0	49
58	A	1665,0	393,0	99
59	A	2885,0	32,0	8
60	A	2890,0	102,0	25
61	A	2982,0	6,0	1
62	A	2983,0	55,0	13
63	A	3017,0	30,0	7
64	A	3033,0	12,0	3
65	A	3040,0	20,0	5
66	A	3065,0	24,0	6
67	A	3104,0	6,0	1
68	A	3125,0	2,0	0
69	A	3475,0	39,0	9

[i] (a) R. N. Veedu, J. O. Kokas, I. Couturier-Tamburelli, R. Koch J.-P. Aycard, F. Borget, and C. Wentrup, *J. Phys Chem. A*, **2008**, *112*, 9742. (b) R. Koch, J. J. Finnerty, T. Bruhn, F. Borget, C. Wentrup, *J. Phys. Chem. A* **2008**, *112*, 8999.