ELECTRONIC SUPPLEMENTARY INFORMATION

Tautomerism in Schiff bases. The cases of 2-hydroxy-1-naphthaldehyde and 1-hydroxy-2-naphthaldehyde investigated in solution and the solid state

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Pages	Supplementary Information

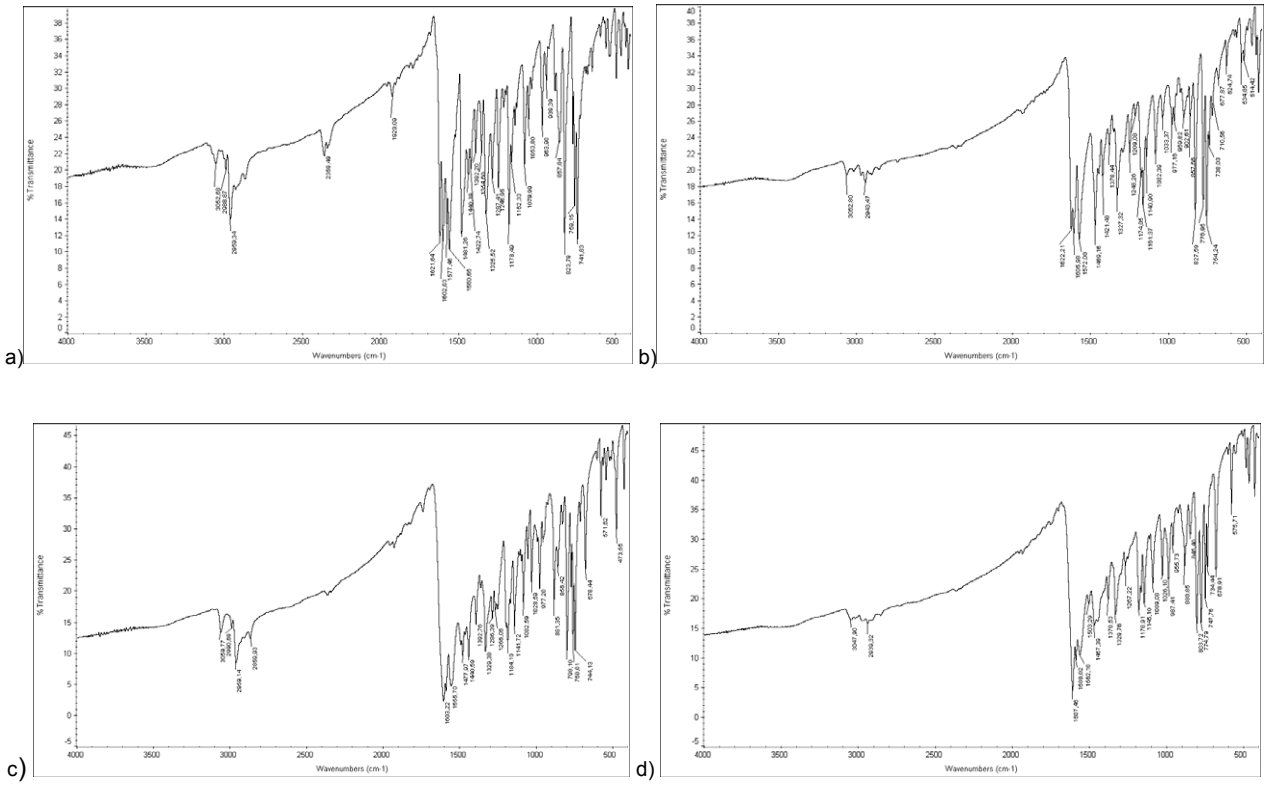

Fig. S1 FT-IR spectra for **25**-**28** (a-d).

Table S1. Selected lengths (Å) and torsion angles (°) for compound **25**.

		Calculated structure					
		Gas phase				Crystal	
Parameter	X-ray data[a]	Imine[b]	Enamine[b]	Imine[c]	Enamine[c]	Imine[b]	Enamine[b]
O1-C9	1.355	1.335	1.263	1.331	1.246	1.338	1.261
N1-C11	1.291	1.298	1.337	1.285	1.330	1.299	1.338
N1-C12	1.425	1.415	1.415	1.415	1.141	1.141	1.141
C9-C10	1.394	1.411	1.463	1.398	1.458	1.411	1.465
C10-C11	1.446	1.447	1.395	1.453	1.387	1.447	1.392
O1-H1/N1-H1	1.044	1.006	1.039	0.995	1.027	1.004	1.034
C11-N1-C12-C13	44.85	47.46	32.54	49.03	38.99	41.64	33.18
N1-C11-C10-C9	0.72	7.11	1.03	4.40	2.04	1.73	3.61
C11-C10-C9-O1	1.65	1.89	2.54	1.65	3.96	2.24	5.20
C10-C9-O1-H1	1.42	0.49	1.58	0.29	1.97	0.25	1.42
C9-O1-H1-N1	0.60	2.32	1.42	0.06	3.30	3.26	7.08
O1-H1-N1-C11	0.18	6.52	2.80	2.31	5.16	3.58	8.81
H1-N1-C11-C10	0.10	7.14	1.26	3.86	2.16	0.10	2.69

[a] At 120 K. [b] At the B3LYP/6-31G** level of theory. [c] At the M06-2X/6-311++G** level of theory.

Table S2. Selected lengths (Å) and torsion angles (°) for compound **26**.

		Calculated structure (gas phase)			
Parameter	X-ray data[a]	Imine[b]	Enamine[b]	Imine[c]	Enamine[c]
O1-C9	1.351	1.334	1.262	1.330	1.245
N1-C11	1.290	1.295	1.336	1.283	1.331
N1-C12	1.423	1.418	1.417	1.416	1.417
C9-C10	1.397	1.412	1.463	1.397	1.458
C10-C11	1.443	1.445	1.396	1.453	1.386
O1-H1/N1-H1	0.904	1.009	1.044	0.996	1.029
C11-N1-C12-C13	49.80	65.90	47.19	58.74	49.12
N1-C11-C10-C9	7.17	0.48	2.99	3.77	5.57
C11-C10-C9-O1	0.55	0.40	1.75	1.42	4.66
C10-C9-O1-H1	1.95	0.15	0.44	1.18	1.70
C9-O1-H1-N1	4.93	0.96	0.37	2.59	1.05
O1-H1-N1-C11	11.20	0.87	1.44	0.58	0.43
H1-N1-C11-C10	8.97	0.10	2.67	2.78	3.30

[a] At 120 K. [b] At the B3LYP/6-31G** level of theory. [c] At the M06-2X/6-311++G** level of theory.

Table S3. Selected lengths (Å) and torsion angles (°) for compound **27**.

		Calculated structure (gas phase)			
Parameter	X-ray data[a]	Imine[b]	Enamine[b]	Imine[c]	Enamine[c]
O1-C1	1.315	1.337	1.260	1.332	1.243
N1-C11	1.305	1.297	1.338	1.282	1.330
N1-C12	1.426	1.415	1.414	1.415	1.414
C1-C10	1.417	1.407	1.460	1.393	1.455
C10-C11	1.421	1.446	1.460	1.452	1.386
O1-H1/N1-H2	0.840/0.880	1.005	1.033	0.991	1.024
C11-N1-C12-C13	36.06	44.25	30.14	48.75	38.73
N1-C11-C10-C1	0.65	1.92	0.11	1.76	0.00
C11-C10-C1-O1	2.62	0.29	1.39	0.28	0.67
C10-C1-O1-H1	14.25	0.46	0.92	0.29	0.18
C1-O1-H1-N1	38.42	3.09	1.23	1.96	2.86
O1-H1-N1-C11	37.88	4.32	2.38	3.54	3.57
H1-N1-C11-C10	7.85	2.49	1.51	2.44	2.00

[a] At 120 K. [b] At the B3LYP/6-31G** level of theory. [c] At the M06-2X/6-311++G** level of theory.

Table S4. Selected lengths (Å) and torsion angles (°) for compound **28**.

		Calculated structure (gas phase)			
Parameter	X-ray data[a]	Imine[b]	Enamine[b]	Imine[c]	Enamine[c]
O1-C1	1.337	1.336	1.259	1.331	1.242
N1-C11	1.289	1.293	1.337	1.281	1.331
N1-C12	1.418	1.418	1.418	1.417	1.418
C1-C10	1.395	1.408	1.461	1.394	1.456
C10-C11	1.445	1.447	1.393	1.452	1.384
O1-H1/N1-H1	1.071	1.006	1.04	0.993	1.027
C11-N1-C12-C13	131.77	117.53	135.73	119.74	132.18
N1-C11-C10-C1	2.44	0.19	1.34	0.08	1.85
C11-C10-C1-O1	2.86	0.03	0.08	0.13	0.11
C10-C1-O1-H1	1.56	0.08	0.08	0.29	0.38
C1-O1-H1-N1	0.20	0.57	2.19	0.39	1.75
O1-H1-N1-C11	0.54	0.73	3.47	0.21	3.49
H1-N1-C11-C10	0.89	0.34	2.75	0.09	3.44

[a] At 120 K. [b] At the B3LYP/6-31G** level of theory. [c] At the M06-2X/6-311++G** level of theory.

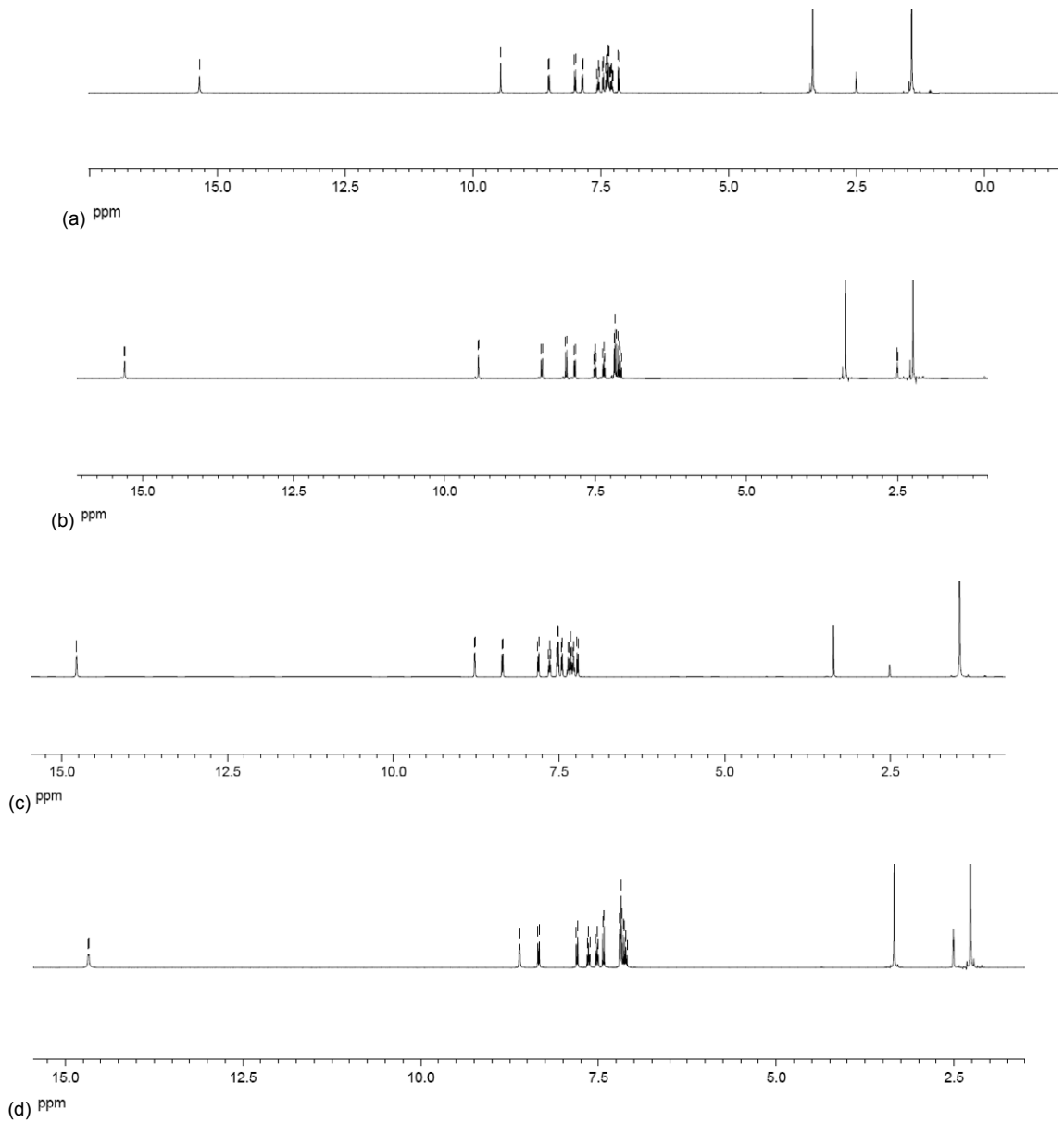

Fig. S2. ^{1}H NMR spectra for **25**(a), **26**(b), **27**(c), and **28**(d).

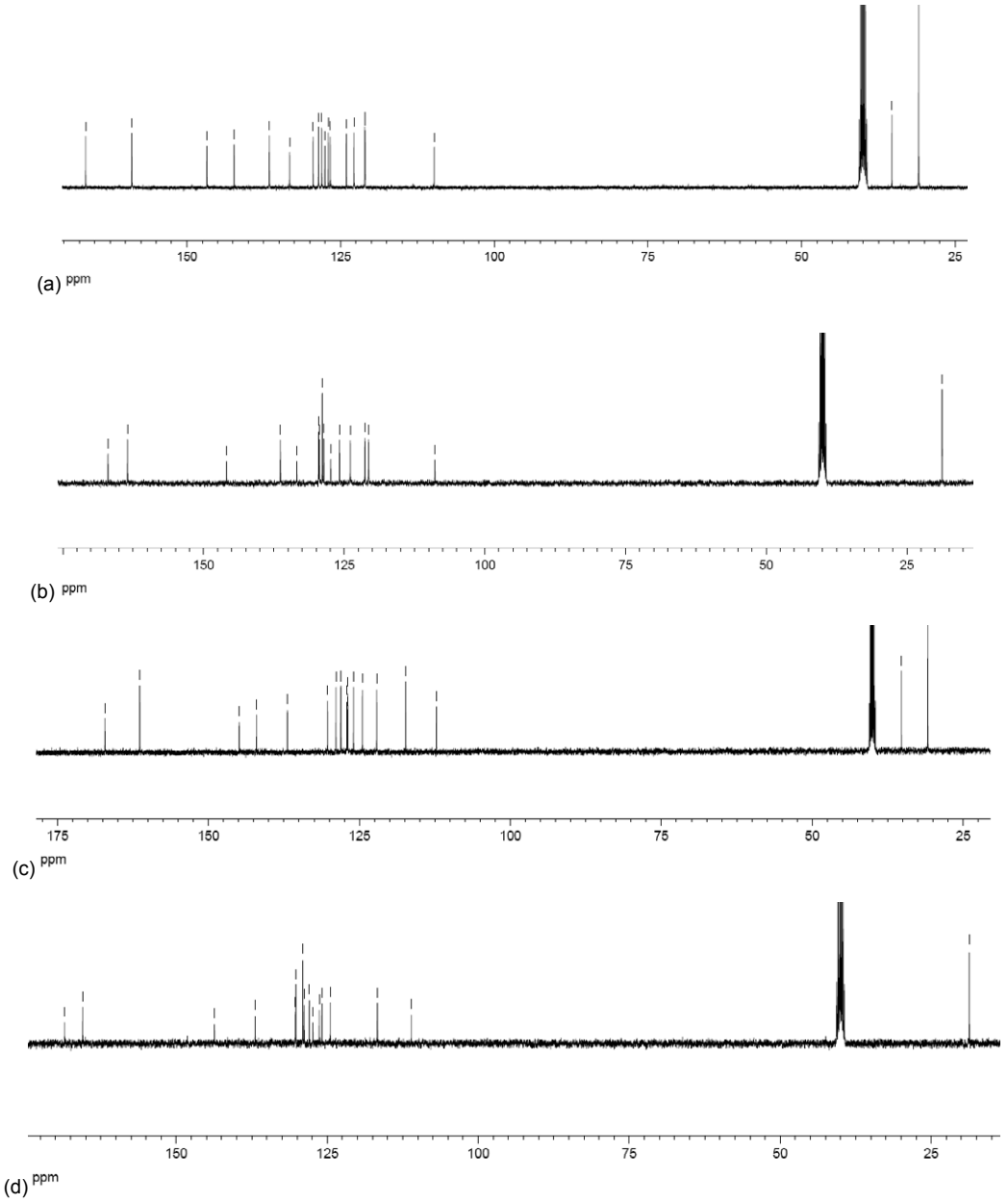

Fig. S3. ^{13}C NMR spectra for **25**(a), **26**(b), **27**(c), and **28**(d).

Table S5. Selected calculated lengths (Å) and torsion angles (°) for compound **25**-**28** in solution.[a]

	25		**26**			**27**		**28**	
Parameter	Imine	Enamine	Imine	Enamine	Parameter	Imine	Enamine	Imine	Enamine
O1-C9	1.334	1.252	1.334	1.251	O1-C1	1.335	1.249	1.334	1.247
N1-C11	1.286	1.325	1.284	1.324	N1-C11	1.283	1.323	1.282	1.323
N1-C12	1.416	1.419	1.417	1.422	N1-C12	1.416	1.419	1.416	1.423
C9-C10	1.397	1.452	1.397	1.452	C9-C10	1.424	1.439	1.424	1.439
C10-C11	1.455	1.395	1.456	1.395	C10-C11	1.455	1.395	1.455	1.395
O1-H1/N1-H1	1.000	1.024	1.002	1.025	O1-H1/N1-H2	0.997	1.022	0.999	1.024
N1-C11-C10-C9	3.37	2.65	1.45	2.76	N1-C11-C10-C1	1.99	0.79	1.19	0.37
C11-C10-C9-O1	1.17	3.79	0.47	2.27	C11-C10-C1-O1	0.24	0.43	0.15	0.03
C10-C9-O1-H1	0.88	1.03	0.10	1.55	C10-C1-O1-H1	1.20	1.10	0.22	1.06
C9-O1-H1-N1	1.62	4.85	0.22	2.06	C1-O1-H1-N1	0.42	4.17	0.43	4.12
O1-H1-N1-C11	0.26	6.15	1.03	2.54	O1-H1-N1-C11	1.43	4.12	1.28	4.67
H1-N1-C11-C10	2.69	2.13	1.37	2.91	H1-N1-C11-C10	2.22	1.53	1.29	2.76

[a] At the M06-2X/6-311++G** level , including the solvent effect (SMD model, DMSO as solvent).

Table S6. Crystal and experimental data for **25**-**28**.

	25	**26**	**27**	**28**
Empirical formula	$C_{21}H_{21}NO$	$C_{19}H_{17}NO$	$C_{21}H_{21}NO$	$C_{19}H_{17}NO$
Formula weight	303.39	275.34	303.39	275.34
Temperature	120(2) K	120(2) K	120(2) K	120(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_12_12_1$	$P2_1/n$	$P2_1$
Unit cell dimensions	a = 8.0440(2) Å	a = 7.6826(2) Å	a = 8.5131(2) Å	a = 8.4367(3) Å
	b = 18.8305(8) Å	b = 12.2144(4) Å	b = 12.4731(4) Å	b = 7.7374(3) Å
	c = 11.1262(4) Å	c = 15.2964(4) Å	c = 15.8417(5) Å	c = 11.1697(5) Å
Volume	1650.08(10) $Å^3$	1435.39(7) $Å^3$	1638.95(8) $Å^3$	729.03(5) $Å^3$
Z	4	4	4	2
Calculated density	1.221 g / cm^3	1.274 g / cm^3	1.230 g / cm^3	1.254 g / cm^3
Absorption coefficient	0.074 mm^{-1}	0.078 mm^{-1}	0.075 mm^{-1}	0.077 mm^{-1}
F(000)	648	584	648	292
Crystal size	0.20 × 0.18 × 0.03 mm^3	0.32 × 0.28 × 0.22 mm^3	0.30 × 0.10 × 0.06 mm^3	0.20 × 0.08 × 0.02 mm^3
θ Range for data collection	3.37 - 27.48°	3.13 - 25.03°	3.10 – 27.48°	3.00 - 27.48°
Limiting indices	$-10 \le h \le 10$, $-24 \le k \le 24$,	$-9 \le h \le 9$, $-14 \le k \le 14$,	$-10 \le h \le 11$, $-16 \le k \le 16$,	$-10 \le h \le 10$, $-9 \le k \le 9$,
	$-14 \le l \le 14$	$-18 \le l \le 18$	$-20 \le l \le 20$	$-14 \le l \le 14$
Reflections collected / unique	24247 / 3779 R_{int} = 0.0866	12111 / 1470 R_{int} = 0.0462	20079 / 3746 R_{int} = 0.0727	8693 / 1772 R_{int} = 0.0461
Completeness to θ = 27.48	99.8 %	99.4 %	99.7 %	99.2 %
Data / restraints / parameters	3779 / 0 / 215	1470 / 1 / 196	3746 / 0 / 215	1772 / 1 / 196
Goodness-of-fit on F^2	1.031	1.189	1.056	1.206
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0583, wR_2 = 0.1378	R_1 = 0.0333, wR_2 = 0.0800	R_1 = 0.0568, wR_2 = 0.1366	R_1 = 0.0538, wR_2 = 0.1057
R indices (all data)	R_1 = 0.1081, wR_2 = 0.1634	R_1 = 0.0366, wR_2 = 0.0819	R_1 = 0.0938, wR_2 = 0.1562	R_1 = 0.0739, wR_2 = 0.1174
Largest diff. peak and hole	0.198 and -0.251 e $Å^{-3}$	0.162 and -0.206 e $Å^{-3}$	0.198 and -0.273 e $Å^{-3}$	0.186 and -0.196 e $Å^{-3}$

COMPUTATIONAL DATA (at the M06-2X/6-311++G** level in gas phase)

Cartesians coordinates for compound **25** (imine form)

E= -942.71625960 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.040920	-0.349762	-0.013137
2	6	0	-5.264591	0.230687	0.393219
3	6	0	-5.304610	1.492533	0.927085
4	6	0	-4.104641	2.215150	1.073570
5	6	0	-2.902488	1.675354	0.685376
6	6	0	-2.826647	0.375442	0.122490
7	6	0	-2.841636	-2.246761	-0.941165
8	6	0	-4.009006	-1.665981	-0.555386
9	6	0	-0.329272	0.474652	-0.229780
10	6	0	-1.593297	-0.237979	-0.303161
11	6	0	-1.618085	-1.538310	-0.814570
12	1	0	-4.944687	-2.206516	-0.652871
13	1	0	-2.800899	-3.248475	-1.350125
14	1	0	-0.339979	1.511511	0.111384
15	1	0	-2.007841	2.265663	0.828588
16	1	0	-6.175121	-0.347408	0.275900
17	1	0	-6.244898	1.930685	1.238104
18	1	0	-4.127342	3.210736	1.501168
19	7	0	0.792634	-0.069060	-0.540693
20	8	0	-0.521006	-2.177002	-1.214334
21	6	0	1.965513	0.722715	-0.513008
22	6	0	3.144783	0.259597	0.113150
23	6	0	1.939671	1.961744	-1.159672
24	6	0	4.244507	1.121109	0.082272
25	6	0	3.056846	2.784637	-1.182493
26	1	0	1.035427	2.255100	-1.680924
27	6	0	4.214276	2.361732	-0.548984

28	1	0	5.165467	0.824931	0.564443
29	1	0	3.020283	3.736385	-1.698730
30	1	0	5.101092	2.984297	-0.549699
31	6	0	3.238399	-1.116113	0.792174
32	6	0	4.578063	-1.294013	1.521882
33	1	0	4.591609	-2.276574	1.998634
34	1	0	5.427491	-1.251574	0.836406
35	1	0	4.717553	-0.540864	2.302028
36	6	0	2.128247	-1.303687	1.843880
37	1	0	2.119035	-0.466151	2.546975
38	1	0	1.140670	-1.390370	1.394764
39	1	0	2.319112	-2.219474	2.409926
40	6	0	3.151674	-2.221547	-0.275347
41	1	0	3.216022	-3.203135	0.202939
42	1	0	2.219136	-2.181757	-0.835568
43	1	0	3.978179	-2.131161	-0.984809
44	1	0	0.248568	-1.563605	-1.069396

Cartesians coordinates for compound **25** (enamine form)

E= -942.71148821 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.062921	-0.403825	-0.048492
2	6	0	-5.322744	0.137124	0.254031
3	6	0	-5.448858	1.426547	0.727336
4	6	0	-4.294677	2.195073	0.911902
5	6	0	-3.047147	1.678454	0.618780
6	6	0	-2.892632	0.369910	0.122209
7	6	0	-2.770145	-2.339251	-0.811035
8	6	0	-3.953208	-1.762822	-0.527907
9	6	0	-0.431754	0.519772	-0.151892
10	6	0	-1.600904	-0.223780	-0.217188
11	6	0	-1.516200	-1.611027	-0.657726

12	1	0	-4.874741	-2.324640	-0.649959
13	1	0	-2.691989	-3.361261	-1.161140
14	1	0	-0.457047	1.561274	0.150009
15	1	0	-2.184183	2.307865	0.795288
16	1	0	-6.201781	-0.482430	0.109308
17	1	0	-6.424034	1.836590	0.958478
18	1	0	-4.374759	3.206166	1.293945
19	7	0	0.779155	0.044899	-0.427730
20	8	0	-0.432475	-2.173544	-0.907440
21	1	0	0.776486	-0.953627	-0.665801
22	6	0	1.966054	0.813900	-0.419072
23	6	0	3.176506	0.277888	0.070988
24	6	0	1.898563	2.114499	-0.920383
25	6	0	4.282437	1.133022	0.038151
26	6	0	3.015320	2.936326	-0.921713
27	1	0	0.965241	2.465501	-1.345293
28	6	0	4.215305	2.438708	-0.437902
29	1	0	5.236070	0.781228	0.405143
30	1	0	2.947713	3.942610	-1.316556
31	1	0	5.105537	3.056094	-0.435473
32	6	0	3.300201	-1.154920	0.619845
33	6	0	4.701151	-1.405636	1.198703
34	1	0	4.739720	-2.420645	1.598954
35	1	0	5.479107	-1.323455	0.435984
36	1	0	4.932334	-0.715313	2.013887
37	6	0	2.298461	-1.400778	1.765911
38	1	0	2.427262	-0.649580	2.549792
39	1	0	1.258752	-1.387193	1.442992
40	1	0	2.489206	-2.384022	2.203904
41	6	0	3.098894	-2.186618	-0.508733
42	1	0	3.281782	-3.189896	-0.113924
43	1	0	2.094464	-2.201126	-0.932557
44	1	0	3.810376	-2.005476	-1.318229

Cartesians coordinates for compound **25** (TS)

E= -942.70824602 HF (976i cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.027622	-0.437655	-0.042645
2	6	0	-5.303238	0.051944	0.300208
3	6	0	-5.464426	1.327091	0.790326
4	6	0	-4.335094	2.145663	0.949660
5	6	0	-3.078067	1.687278	0.620720
6	6	0	-2.884615	0.383331	0.113411
7	6	0	-2.661143	-2.279777	-0.888254
8	6	0	-3.869574	-1.770681	-0.552144
9	6	0	-0.396366	0.598347	-0.145542
10	6	0	-1.591208	-0.152473	-0.251538
11	6	0	-1.468176	-1.487226	-0.744020
12	1	0	-4.762906	-2.377869	-0.663401
13	1	0	-2.542729	-3.285801	-1.271067
14	1	0	-0.404590	1.622882	0.220585
15	1	0	-2.235392	2.351609	0.764294
16	1	0	-6.160711	-0.600038	0.169618
17	1	0	-6.447841	1.696721	1.052470
18	1	0	-4.450312	3.150890	1.338234
19	7	0	0.755685	0.068944	-0.466796
20	8	0	-0.329098	-1.986069	-1.055345
21	6	0	1.964624	0.805058	-0.432307
22	6	0	3.148068	0.255233	0.106461
23	6	0	1.945429	2.097368	-0.961982
24	6	0	4.271651	1.087915	0.099119
25	6	0	3.080398	2.894038	-0.948925
26	1	0	1.031137	2.458926	-1.418728
27	6	0	4.250532	2.382765	-0.409995
28	1	0	5.203629	0.724948	0.508890
29	1	0	3.048968	3.892077	-1.368595
30	1	0	5.153822	2.980727	-0.390529
31	6	0	3.227637	-1.173256	0.669449

32	6	0	4.589503	-1.438854	1.328408
33	1	0	4.592288	-2.453402	1.732197
34	1	0	5.411468	-1.369446	0.612280
35	1	0	4.782030	-0.748510	2.153871
36	6	0	2.156764	-1.412553	1.751855
37	1	0	2.227036	-0.650876	2.533396
38	1	0	1.142821	-1.412218	1.356616
39	1	0	2.326560	-2.388444	2.214339
40	6	0	3.074674	-2.191995	-0.475806
41	1	0	3.165499	-3.205880	-0.075835
42	1	0	2.112830	-2.130382	-0.982385
43	1	0	3.862772	-2.046405	-1.219149
44	1	0	0.508088	-1.032914	-0.815539

Cartesians coordinates for compound **26** (imine form)

E= -864.11320903 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.622038	0.207903	-0.032857
2	6	0	-4.772320	-0.573173	-0.290469
3	6	0	-4.663870	-1.887260	-0.665592
4	6	0	-3.384530	-2.463353	-0.790501
5	6	0	-2.251111	-1.726213	-0.547915
6	6	0	-2.327666	-0.361834	-0.165991
7	6	0	-2.650360	2.332494	0.632930
8	6	0	-3.743988	1.568870	0.368554
9	6	0	0.175092	-0.066647	-0.057431
10	6	0	-1.171521	0.455442	0.101702
11	6	0	-1.347853	1.781380	0.506034
12	1	0	-4.738619	1.991470	0.466150
13	1	0	-2.729047	3.366581	0.944122
14	1	0	0.292761	-1.075357	-0.456369
15	1	0	-1.292253	-2.216367	-0.649670
16	1	0	-5.746929	-0.108841	-0.181385
17	1	0	-5.548873	-2.479664	-0.862212

18	1	0	-3.291023	-3.503377	-1.080526
19	7	0	1.221353	0.619693	0.226188
20	8	0	-0.331906	2.594273	0.782833
21	6	0	2.500112	0.031871	0.070317
22	6	0	3.421217	0.706618	-0.747075
23	6	0	2.854259	-1.138605	0.759840
24	6	0	4.693107	0.166711	-0.905595
25	6	0	4.146058	-1.637713	0.583322
26	6	0	5.057350	-1.003035	-0.247800
27	1	0	5.405866	0.674334	-1.546397
28	1	0	4.437371	-2.534448	1.119901
29	1	0	6.054105	-1.409435	-0.371456
30	1	0	0.510407	2.076533	0.665289
31	6	0	3.015682	1.978080	-1.442489
32	1	0	2.194076	1.802063	-2.141239
33	1	0	2.665277	2.721404	-0.721970
34	1	0	3.855518	2.399047	-1.995609
35	6	0	1.910502	-1.830165	1.714992
36	1	0	1.302044	-1.110980	2.266166
37	1	0	1.227419	-2.512210	1.201386
38	1	0	2.478953	-2.421021	2.433988

Cartesians coordinates for compound **26** (enamine form)

E= -864.10894057 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.632097	0.261326	-0.094436
2	6	0	-4.799447	-0.473413	-0.356422
3	6	0	-4.744982	-1.827399	-0.615647
4	6	0	-3.502471	-2.469811	-0.602080
5	6	0	-2.344130	-1.761626	-0.344336
6	6	0	-2.370920	-0.375280	-0.100018
7	6	0	-2.628545	2.419162	0.487005
8	6	0	-3.712594	1.674544	0.200875
9	6	0	0.088642	-0.126614	0.041870

10	6	0	-1.177126	0.423307	0.167053
11	6	0	-1.289043	1.839187	0.498544
12	1	0	-4.698565	2.130285	0.194744
13	1	0	-2.695389	3.475653	0.716632
14	1	0	0.209650	-1.138935	-0.325419
15	1	0	-1.409243	-2.307854	-0.318692
16	1	0	-5.752300	0.045644	-0.347473
17	1	0	-5.649933	-2.386848	-0.817163
18	1	0	-3.444037	-3.536145	-0.786836
19	7	0	1.225466	0.513702	0.304094
20	8	0	-0.300980	2.550836	0.755598
21	1	0	1.088017	1.498189	0.570511
22	6	0	2.524510	-0.011985	0.091693
23	6	0	3.446545	0.819934	-0.564359
24	6	0	2.878123	-1.288852	0.549701
25	6	0	4.728342	0.334703	-0.795609
26	6	0	4.173014	-1.738184	0.285115
27	6	0	5.090633	-0.943620	-0.385349
28	1	0	5.446103	0.965497	-1.307992
29	1	0	4.465114	-2.722420	0.635058
30	1	0	6.091538	-1.312601	-0.574235
31	6	0	3.039540	2.199521	-1.009809
32	1	0	2.150554	2.163300	-1.644545
33	1	0	2.794949	2.841594	-0.158286
34	1	0	3.846672	2.674491	-1.566838
35	6	0	1.942886	-2.158169	1.354999
36	1	0	1.267941	-1.560588	1.970409
37	1	0	1.331460	-2.806112	0.720137
38	1	0	2.521755	-2.806149	2.013813

Cartesians coordinates for compound **26** (TS)

E= -864.10530895 HF (1011i cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.630393	0.297286	0.035402

2	6	0	-4.841574	-0.386394	-0.189392
3	6	0	-4.848764	-1.694678	-0.613219
4	6	0	-3.625746	-2.352700	-0.821321
5	6	0	-2.429501	-1.704315	-0.604867
6	6	0	-2.393247	-0.360618	-0.170784
7	6	0	-2.491503	2.357956	0.691236
8	6	0	-3.633340	1.665199	0.470859
9	6	0	0.111727	-0.206681	-0.092610
10	6	0	-1.169854	0.371476	0.073358
11	6	0	-1.207860	1.735513	0.496683
12	1	0	-4.595778	2.144958	0.621653
13	1	0	-2.494838	3.390789	1.017047
14	1	0	0.226848	-1.233211	-0.432645
15	1	0	-1.509793	-2.248729	-0.778665
16	1	0	-5.774437	0.142011	-0.022188
17	1	0	-5.783755	-2.213021	-0.785404
18	1	0	-3.619912	-3.383395	-1.156690
19	7	0	1.190283	0.491100	0.146542
20	8	0	-0.136372	2.408013	0.701530
21	6	0	2.504021	-0.024407	0.039645
22	6	0	3.432437	0.748608	-0.676941
23	6	0	2.872203	-1.224109	0.666344
24	6	0	4.733307	0.275185	-0.802700
25	6	0	4.190573	-1.658854	0.517019
26	6	0	5.112671	-0.927529	-0.216208
27	1	0	5.455187	0.858017	-1.364012
28	1	0	4.494515	-2.579986	1.002618
29	1	0	6.130471	-1.284714	-0.317377
30	1	0	0.811027	1.573548	0.456301
31	6	0	3.006799	2.052234	-1.297508
32	1	0	2.184727	1.902894	-2.001851
33	1	0	2.650917	2.754637	-0.539181
34	1	0	3.839465	2.514057	-1.827870
35	6	0	1.923643	-2.019941	1.530306
36	1	0	1.366151	-2.762927	0.953059
37	1	0	2.485679	-2.559442	2.293349
38	1	0	1.198939	-1.376681	2.032001

Cartesians coordinates for compound **27** (imine form)

E= -942.72059828 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.180033	-1.297734	0.238697
2	1	0	-0.553109	-2.205336	0.727978
3	7	0	-0.992435	-0.470137	-0.308623
4	6	0	-2.373423	-0.779620	-0.337774
5	6	0	-3.342008	0.181163	0.031129
6	6	0	-2.758446	-2.049308	-0.777562
7	6	0	-4.676856	-0.227158	-0.027378
8	6	0	-4.095679	-2.414611	-0.836748
9	6	0	-5.059543	-1.497303	-0.450265
10	1	0	-5.457155	0.461546	0.264559
11	1	0	-4.375392	-3.400261	-1.188637
12	1	0	-6.111026	-1.756618	-0.483814
13	6	0	-2.970150	1.607666	0.466369
14	6	0	1.254715	-1.078564	0.278871
15	6	0	2.091696	-2.016385	0.946884
16	6	0	1.826534	0.043841	-0.317737
17	6	0	3.440393	-1.844450	1.017787
18	1	0	1.625173	-2.881739	1.406665
19	6	0	3.239785	0.246203	-0.261799
20	6	0	4.046066	-0.705086	0.412207
21	1	0	4.067287	-2.563952	1.530731
22	6	0	3.836476	1.377901	-0.865751
23	6	0	5.444148	-0.487048	0.461904
24	6	0	5.194386	1.559151	-0.800140
25	1	0	3.199857	2.089517	-1.375911
26	6	0	6.004494	0.617102	-0.128973
27	1	0	6.065610	-1.210917	0.977593
28	1	0	5.650183	2.425916	-1.263149
29	1	0	7.076388	0.770032	-0.082269
30	8	0	1.097550	0.960503	-0.952935
31	1	0	0.149687	0.675699	-0.895255
32	1	0	-1.989489	-2.738395	-1.108074
33	6	0	-4.199251	2.387467	0.956124

34	1	0	-4.950297	2.506427	0.171862
35	1	0	-4.666450	1.906918	1.819961
36	1	0	-3.883055	3.387805	1.259868
37	6	0	-2.396385	2.374607	-0.738553
38	1	0	-2.094704	3.379256	-0.428863
39	1	0	-1.527784	1.878543	-1.168568
40	1	0	-3.152607	2.470106	-1.522022
41	6	0	-1.956753	1.599382	1.626828
42	1	0	-2.316601	0.972413	2.447483
43	1	0	-0.976242	1.239669	1.321442
44	1	0	-1.834629	2.617007	2.007535

Cartesians coordinates for compound **27** (enamine form)

E= -942.71708599 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.096940	-1.421820	0.202623
2	1	0	-0.470554	-2.365522	0.592983
3	7	0	-1.012686	-0.567605	-0.245496
4	6	0	-2.404284	-0.815208	-0.285317
5	6	0	-3.333040	0.205480	0.010807
6	6	0	-2.823838	-2.098992	-0.636895
7	6	0	-4.681850	-0.157597	-0.052136
8	6	0	-4.171211	-2.422786	-0.672669
9	6	0	-5.105446	-1.442457	-0.376789
10	1	0	-5.440460	0.579758	0.167876
11	1	0	-4.481617	-3.422618	-0.950220
12	1	0	-6.165060	-1.665686	-0.405356
13	6	0	-2.916547	1.639578	0.385461
14	6	0	1.265254	-1.169021	0.224943
15	6	0	2.166998	-2.164038	0.748560
16	6	0	1.777287	0.102532	-0.264138
17	6	0	3.500124	-1.964720	0.790138
18	1	0	1.741468	-3.094225	1.113722
19	6	0	3.238624	0.285877	-0.212704

20	6	0	4.071457	-0.727806	0.303693
21	1	0	4.166115	-2.722980	1.184426
22	6	0	3.792850	1.483077	-0.684489
23	6	0	5.459578	-0.503604	0.331455
24	6	0	5.158804	1.683091	-0.649362
25	1	0	3.118153	2.236224	-1.073616
26	6	0	5.993882	0.680638	-0.136777
27	1	0	6.108962	-1.277425	0.726452
28	1	0	5.584986	2.608942	-1.016586
29	1	0	7.066363	0.835584	-0.108273
30	8	0	1.031665	0.997274	-0.699896
31	1	0	-0.616682	0.325938	-0.550095
32	1	0	-2.080649	-2.835733	-0.918455
33	6	0	-4.138572	2.485343	0.776631
34	1	0	-4.839071	2.601739	-0.053559
35	1	0	-4.670164	2.056674	1.629907
36	1	0	-3.798764	3.482835	1.062109
37	6	0	-2.260091	2.344153	-0.819309
38	1	0	-2.070336	3.390326	-0.563942
39	1	0	-1.300252	1.923328	-1.121065
40	1	0	-2.930383	2.320654	-1.682089
41	6	0	-1.970598	1.647608	1.603767
42	1	0	-2.437200	1.133657	2.448376
43	1	0	-1.004315	1.185334	1.409953
44	1	0	-1.779716	2.682270	1.900140

Cartesians coordinates for compound **27** (TS)

E= -942.71242971 HF (1074i cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.139572	-1.461354	0.299220
2	1	0	-0.544581	-2.371921	0.743676
3	7	0	-0.952538	-0.586840	-0.228994
4	6	0	-2.349954	-0.799549	-0.311839
5	6	0	-3.269563	0.219409	0.016680

6	6	0	-2.786133	-2.055862	-0.738923
7	6	0	-4.622653	-0.117265	-0.084291
8	6	0	-4.137824	-2.352499	-0.825520
9	6	0	-5.060622	-1.374120	-0.490754
10	1	0	-5.372725	0.618900	0.167379
11	1	0	-4.459956	-3.329764	-1.163744
12	1	0	-6.123072	-1.577008	-0.551087
13	6	0	1.254946	-1.217379	0.321503
14	6	0	2.171783	-2.140760	0.912588
15	6	0	1.720728	-0.005527	-0.261193
16	6	0	3.504521	-1.893461	0.928695
17	1	0	1.774515	-3.051541	1.350235
18	6	0	3.146538	0.252560	-0.248998
19	6	0	4.021968	-0.687473	0.343806
20	1	0	4.198184	-2.595491	1.375705
21	6	0	3.655211	1.431499	-0.825507
22	6	0	5.405028	-0.405408	0.339425
23	6	0	5.008643	1.679918	-0.817746
24	1	0	2.953399	2.127020	-1.269667
25	6	0	5.887412	0.751452	-0.229033
26	1	0	6.085791	-1.119186	0.790756
27	1	0	5.400561	2.586949	-1.261756
28	1	0	6.952994	0.950146	-0.224117
29	8	0	0.903596	0.837002	-0.781114
30	1	0	-0.243346	0.299739	-0.612335
31	1	0	-2.046038	-2.790311	-1.035732
32	6	0	-2.836704	1.627800	0.456144
33	6	0	-4.040566	2.463779	0.916984
34	1	0	-4.762229	2.625098	0.112988
35	1	0	-4.554205	2.000579	1.763696
36	1	0	-3.684502	3.445059	1.237243
37	6	0	-2.201203	2.368153	-0.735080
38	1	0	-1.902674	3.373026	-0.423310
39	1	0	-1.313183	1.873213	-1.125463
40	1	0	-2.924934	2.463413	-1.548721
41	6	0	-1.856158	1.574633	1.645008
42	1	0	-0.882579	1.167477	1.379613
43	1	0	-1.693455	2.588550	2.019809
44	1	0	-2.273929	0.976628	2.459692

Cartesians coordinates for compound **28** (imine form)

E= -864.11736133 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.645671	-0.691678	-0.472412
2	1	0	1.122997	-1.514760	-1.017423
3	7	0	1.354007	0.207296	0.102291
4	6	0	2.767493	0.108267	0.067040
5	6	0	3.474636	1.157884	-0.539225
6	6	0	3.431212	-0.966457	0.677349
7	6	0	4.864025	1.095178	-0.566772
8	6	0	4.826041	-0.983831	0.637885
9	6	0	5.541191	0.028918	0.014571
10	1	0	5.418022	1.895709	-1.045226
11	1	0	5.352936	-1.803218	1.115423
12	1	0	6.623858	-0.004023	-0.005891
13	6	0	2.727128	2.310026	-1.154326
14	1	0	2.089787	1.974661	-1.976363
15	1	0	2.072471	2.785846	-0.419833
16	1	0	3.421143	3.057610	-1.539037
17	6	0	2.680627	-2.055361	1.405352
18	1	0	1.839993	-1.646871	1.969679
19	1	0	2.279528	-2.807338	0.720788
20	1	0	3.346899	-2.567304	2.100209
21	6	0	-0.806357	-0.675115	-0.453763
22	6	0	-1.531626	-1.706486	-1.113738
23	6	0	-1.501225	0.340410	0.201672
24	6	0	-2.893089	-1.728790	-1.119682
25	1	0	-0.969624	-2.485215	-1.619606
26	6	0	-2.930420	0.340018	0.211052
27	6	0	-3.624358	-0.702249	-0.454177
28	1	0	-3.435046	-2.519108	-1.625383
29	6	0	-3.653121	1.360800	0.872538
30	6	0	-5.040016	-0.687050	-0.434339
31	6	0	-5.024672	1.345967	0.872957
32	1	0	-3.100887	2.145610	1.373790
33	6	0	-5.723362	0.311147	0.212511

34	1	0	-5.575583	-1.482148	-0.941813
35	1	0	-5.576103	2.128247	1.380525
36	1	0	-6.807034	0.308464	0.218506
37	8	0	-0.881960	1.335335	0.833705
38	1	0	0.095604	1.190488	0.739028

Cartesians coordinates for compound **28** (enamine form)

E= -864.11432227 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.568477	0.849946	-0.319594
2	1	0	-1.060398	1.721685	-0.742977
3	7	0	-1.370551	-0.110119	0.136013
4	6	0	-2.786907	-0.098094	0.071531
5	6	0	-3.410974	-1.263465	-0.403465
6	6	0	-3.526250	1.013444	0.497870
7	6	0	-4.798314	-1.284620	-0.486681
8	6	0	-4.916433	0.951292	0.384763
9	6	0	-5.551473	-0.179053	-0.106817
10	1	0	-5.290241	-2.176093	-0.859449
11	1	0	-5.504312	1.802454	0.711340
12	1	0	-6.631992	-0.205971	-0.180068
13	6	0	-2.583602	-2.451822	-0.816725
14	1	0	-1.827526	-2.169414	-1.553486
15	1	0	-2.052289	-2.887375	0.035027
16	1	0	-3.217335	-3.226697	-1.247046
17	6	0	-2.887573	2.232773	1.116870
18	1	0	-1.978680	1.977492	1.664215
19	1	0	-2.626977	2.986273	0.368223
20	1	0	-3.585861	2.697426	1.813627
21	6	0	0.814741	0.794227	-0.305584
22	6	0	1.578588	1.904338	-0.817547
23	6	0	1.489996	-0.393601	0.198717
24	6	0	2.926907	1.892589	-0.835027
25	1	0	1.033980	2.766108	-1.192327

26	6	0	2.964554	-0.372448	0.169737
27	6	0	3.656723	0.746828	-0.335846
28	1	0	3.487422	2.736001	-1.220270
29	6	0	3.671755	-1.481547	0.651066
30	6	0	5.062619	0.717088	-0.342350
31	6	0	5.052833	-1.490659	0.636844
32	1	0	3.102609	-2.321938	1.030222
33	6	0	5.748668	-0.381993	0.136076
34	1	0	5.603901	1.573523	-0.729895
35	1	0	5.597656	-2.349506	1.009801
36	1	0	6.832546	-0.386955	0.123561
37	8	0	0.869353	-1.381583	0.624370
38	1	0	-0.867766	-0.944845	0.459426

Cartesians coordinates for compound **28** (TS)

E= -864.10961263 HF (1032i cm^{-1})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.588543	0.979834	-0.405622
2	1	0	-1.082338	1.855125	-0.828120
3	7	0	-1.300270	-0.020141	0.037816
4	6	0	-2.713433	-0.071233	0.031931
5	6	0	-3.293574	-1.270362	-0.417258
6	6	0	-3.498416	0.993238	0.499747
7	6	0	-4.679365	-1.369480	-0.444594
8	6	0	-4.886466	0.847416	0.457373
9	6	0	-5.477304	-0.313243	-0.018056
10	1	0	-5.135301	-2.286171	-0.802038
11	1	0	-5.507192	1.658933	0.821823
12	1	0	-6.556720	-0.403362	-0.040099
13	6	0	-2.417614	-2.410487	-0.863440
14	1	0	-1.751618	-2.103662	-1.673690
15	1	0	-1.781831	-2.764222	-0.047393
16	1	0	-3.025182	-3.246420	-1.209695
17	6	0	-2.909021	2.250053	1.093296

18	1	0	-1.963820	2.052919	1.602046
19	1	0	-2.727182	3.016610	0.334834
20	1	0	-3.604066	2.672587	1.819665
21	6	0	0.826253	0.914710	-0.365280
22	6	0	1.643378	1.992196	-0.826732
23	6	0	1.417262	-0.279961	0.134661
24	6	0	2.996485	1.913186	-0.793043
25	1	0	1.153516	2.883879	-1.206093
26	6	0	2.863870	-0.362726	0.165574
27	6	0	3.637680	0.728831	-0.292871
28	1	0	3.613225	2.733485	-1.139930
29	6	0	3.493097	-1.524063	0.651939
30	6	0	5.044053	0.615714	-0.245686
31	6	0	4.866090	-1.607725	0.685874
32	1	0	2.867412	-2.339292	0.994192
33	6	0	5.644635	-0.526509	0.232862
34	1	0	5.647323	1.447468	-0.593217
35	1	0	5.349511	-2.501630	1.060864
36	1	0	6.726103	-0.594942	0.261323
37	8	0	0.695026	-1.260560	0.540069
38	1	0	-0.494571	-0.852162	0.376213

Simulation of crystal lattices for compound **25** (at the B3LYP/6-31G** level):

Molecular cluster for compound **25** incorporating six molecules in imine form:

E= -5656.12348406 HF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.518535	-1.426872	-0.852949
2	1	0	0.995439	-0.677527	-0.426706
3	7	0	0.503313	0.120917	0.914676
4	6	0	2.720494	-2.408666	2.510257
5	6	0	2.676945	-2.081188	3.891690
6	1	0	2.114164	-1.219641	4.232022
7	6	0	3.349752	-2.835953	4.832200
8	1	0	3.295885	-2.553644	5.879637
9	6	0	4.104325	-3.963755	4.449976
10	1	0	4.625600	-4.551466	5.198978
11	6	0	4.174925	-4.305506	3.117226
12	1	0	4.748360	-5.172082	2.800528
13	6	0	3.502768	-3.545982	2.128185
14	6	0	3.597407	-3.896494	0.749464
15	1	0	4.212930	-4.746838	0.469178
16	6	0	2.945220	-3.183335	-0.217924
17	1	0	3.017792	-3.442899	-1.268128
18	6	0	2.143025	-2.067764	0.137492
19	6	0	2.019170	-1.665720	1.485324
20	6	0	1.158375	-0.552540	1.813071
21	1	0	1.050236	-0.280244	2.865424
22	6	0	-0.443413	1.088670	1.321739
23	6	0	-1.285022	0.776922	2.406573
24	1	0	-1.208630	-0.207530	2.856719
25	6	0	-2.241642	1.673259	2.868366
26	1	0	-2.882811	1.404581	3.702644
27	6	0	-2.374125	2.901625	2.229702
28	1	0	-3.125988	3.612590	2.557198
29	6	0	-1.564650	3.202285	1.131205
30	1	0	-1.705052	4.160513	0.649690

31	6	0	-0.591320	2.324287	0.630879
32	6	0	0.258030	2.722455	-0.598693
33	6	0	-0.081211	1.809684	-1.802133
34	1	0	0.522927	2.100831	-2.668653
35	1	0	-1.134855	1.905253	-2.080411
36	1	0	0.114497	0.756657	-1.602326
37	6	0	1.768186	2.631855	-0.279511
38	1	0	2.024283	3.265899	0.574755
39	1	0	2.345660	2.985658	-1.138847
40	1	0	2.084456	1.612717	-0.057834
41	6	0	-0.019692	4.175577	-1.043551
42	1	0	0.211304	4.896604	-0.253411
43	1	0	-1.056364	4.332134	-1.359530
44	1	0	0.620125	4.414998	-1.897756
45	8	0	10.444591	-3.098353	1.694546
46	1	0	9.740951	-3.529952	1.054647
47	7	0	9.203053	-3.911472	-0.388831
48	6	0	12.336448	-2.181329	-1.350055
49	6	0	12.323954	-2.219809	-2.763261
50	1	0	11.600984	-2.641692	-3.211051
51	6	0	13.334770	-1.657592	-3.502323
52	1	0	13.300557	-1.697640	-4.450875
53	6	0	14.415326	-1.029502	-2.876673
54	1	0	15.112432	-0.644176	-3.394207
55	6	0	14.455741	-0.976910	-1.518311
56	1	0	15.189105	-0.547038	-1.094900
57	6	0	13.440931	-1.543584	-0.722188
58	6	0	13.492203	-1.486701	0.685335
59	1	0	14.239442	-1.072567	1.102264
60	6	0	12.516298	-2.000512	1.462521
61	1	0	12.578960	-1.942507	2.408358
62	6	0	11.402151	-2.622942	0.861684
63	6	0	11.293324	-2.739684	-0.523324
64	6	0	10.153740	-3.413057	-1.105840
65	1	0	10.101935	-3.491089	-2.050540
66	6	0	8.070428	-4.489572	-1.031374
67	6	0	7.491238	-3.800343	-2.099624
68	1	0	7.868436	-2.974676	-2.380872
69	6	0	6.380326	-4.299479	-2.756646
70	1	0	6.002461	-3.828146	-3.489170
71	6	0	5.829749	-5.489528	-2.330384
72	1	0	5.066473	-5.846784	-2.770407
73	6	0	6.393641	-6.165003	-1.258484
74	1	0	5.999540	-6.983503	-0.981252

75	6	0	7.513705	-5.700542	-0.567742
76	6	0	8.081978	-6.479305	0.631101
77	6	0	7.903214	-5.655053	1.916545
78	1	0	8.352815	-6.107161	2.659680
79	1	0	6.947984	-5.566561	2.116288
80	1	0	8.294094	-4.765013	1.790342
81	6	0	9.569918	-6.810730	0.422699
82	1	0	9.681428	-7.305151	-0.416208
83	1	0	9.889836	-7.359920	1.170768
84	1	0	10.088589	-5.980123	0.384461
85	6	0	7.358223	-7.814425	0.846080
86	1	0	7.447433	-8.367020	0.041783
87	1	0	6.408138	-7.646754	1.024093
88	1	0	7.756762	-8.282448	1.610217
89	8	0	5.428344	3.966088	1.902158
90	1	0	6.003404	3.323494	1.313104
91	7	0	6.497621	2.770880	-0.089769
92	6	0	4.171734	5.405717	-1.266048
93	6	0	4.279436	5.347862	-2.675379
94	1	0	4.859975	4.709980	-3.071884
95	6	0	3.563042	6.194950	-3.482118
96	1	0	3.656204	6.134646	-4.425146
97	6	0	2.698846	7.145335	-2.933124
98	1	0	2.204059	7.729567	-3.497919
99	6	0	2.572781	7.226349	-1.580767
100	1	0	1.987797	7.874710	-1.209308
101	6	0	3.287007	6.373644	-0.717410
102	6	0	3.149083	6.461350	0.683551
103	1	0	2.545390	7.099382	1.047266
104	6	0	3.845037	5.671016	1.525703
105	1	0	3.732013	5.757622	2.465466
106	6	0	4.742751	4.714652	1.005048
107	6	0	4.912902	4.551662	-0.368979
108	6	0	5.815902	3.539832	-0.870972
109	1	0	5.912100	3.437759	-1.810795
110	6	0	7.430165	1.849710	-0.651455
111	6	0	8.279515	2.302244	-1.663540
112	1	0	8.211147	3.202467	-1.961679
113	6	0	9.218235	1.464389	-2.239423
114	1	0	9.782944	1.779803	-2.935417
115	6	0	9.321935	0.165516	-1.787550
116	1	0	9.960981	-0.423305	-2.172848
117	6	0	8.489099	-0.278482	-0.770274
118	1	0	8.577072	-1.177532	-0.474575

119	6	0	7.529170	0.530363	-0.162941
120	6	0	6.650470	-0.007426	0.979612
121	6	0	6.987081	0.730644	2.284486
122	1	0	6.360324	0.457529	2.985893
123	1	0	7.900203	0.509045	2.559876
124	1	0	6.913502	1.697785	2.141573
125	6	0	5.155796	0.156234	0.655260
126	1	0	4.956524	-0.294190	-0.203651
127	1	0	4.616782	-0.247854	1.374943
128	1	0	4.936865	1.108196	0.586132
129	6	0	6.887864	-1.502024	1.232497
130	1	0	6.687506	-2.006735	0.416847
131	1	0	7.823772	-1.646897	1.484574
132	1	0	6.301974	-1.806186	1.958065
133	8	0	-5.602741	-5.946270	-2.215891
134	1	0	-4.899225	-5.515571	-1.576519
135	7	0	-4.361111	-5.133235	-0.132532
136	6	0	-7.494659	-6.863273	0.828801
137	6	0	-7.482283	-6.825629	2.241474
138	1	0	-6.759207	-6.402909	2.689794
139	6	0	-8.492986	-7.387012	2.981063
140	1	0	-8.458890	-7.347806	3.929088
141	6	0	-9.573542	-8.015113	2.355412
142	1	0	-10.270876	-8.401794	2.873259
143	6	0	-9.613956	-8.067702	0.997051
144	1	0	-10.347318	-8.497569	0.573645
145	6	0	-8.599248	-7.501854	0.200416
146	6	0	-8.650539	-7.558743	-1.207110
147	1	0	-9.397766	-7.972870	-1.624047
148	6	0	-7.674623	-7.044926	-1.984294
149	1	0	-7.737177	-7.102098	-2.929603
150	6	0	-6.560331	-6.421672	-1.382973
151	6	0	-6.451628	-6.305767	0.001507
152	6	0	-5.312055	-5.632440	0.583926
153	1	0	-5.260235	-5.554317	1.528731
154	6	0	-3.228651	-4.555109	0.510036
155	6	0	-2.649543	-5.244245	1.578624
156	1	0	-3.026811	-6.069729	1.859719
157	6	0	-1.538492	-4.746469	2.234972
158	1	0	-1.160879	-5.216334	2.968226
159	6	0	-0.986584	-3.555569	1.807654
160	1	0	-0.226234	-3.200091	2.243011
161	6	0	-1.551196	-2.878670	0.739886
162	1	0	-1.156960	-2.059186	0.464236

163	6	0	-2.672092	-3.343903	0.046991
164	6	0	-3.240416	-2.566759	-1.151945
165	6	0	-3.061346	-3.389761	-2.437696
166	1	0	-3.511173	-2.938339	-3.181427
167	1	0	-2.106439	-3.478306	-2.638556
168	1	0	-3.452381	-4.280547	-2.312141
169	6	0	-4.728209	-2.233949	-0.944068
170	1	0	-4.839628	-1.739449	-0.105124
171	1	0	-5.048138	-1.685556	-1.692717
172	1	0	-5.246818	-3.064494	-0.905791
173	6	0	-2.516368	-1.230947	-1.367680
174	1	0	-2.605781	-0.677213	-0.562706
175	1	0	-1.566118	-1.399180	-1.544502
176	1	0	-2.915133	-0.763621	-2.131405
177	8	0	-8.118089	-0.022124	0.963388
178	1	0	-8.822722	-0.453488	0.323423
179	7	0	-9.359669	-0.835236	-1.120061
180	6	0	-6.226169	0.894876	-2.081355
181	6	0	-6.238677	0.856402	-3.494513
182	1	0	-6.961643	0.434538	-3.942285
183	6	0	-5.228842	1.418791	-4.233613
184	1	0	-5.263061	1.378771	-5.182152
185	6	0	-4.148296	2.046869	-3.607968
186	1	0	-3.451189	2.432222	-4.125472
187	6	0	-4.106894	2.099296	-2.249562
188	1	0	-3.374519	2.529324	-1.826176
189	6	0	-5.121739	1.532600	-1.453569
190	6	0	-5.070387	1.589603	-0.045967
191	1	0	-4.323215	2.003680	0.370880
192	6	0	-6.047325	1.075862	0.731180
193	1	0	-5.984646	1.133868	1.677046
194	6	0	-7.161476	0.453428	0.130410
195	6	0	-7.270303	0.336688	-1.254596
196	6	0	-8.409859	-0.336652	-1.837008
197	1	0	-8.460707	-0.414894	-2.781762
198	6	0	-10.493209	-1.413132	-1.762613
199	6	0	-11.071396	-0.724044	-2.830950
200	1	0	-10.694195	0.101488	-3.112062
201	6	0	-12.183059	-1.222958	-3.488141
202	1	0	-12.561146	-0.751841	-4.220433
203	6	0	-12.733868	-2.413356	-3.062034
204	1	0	-13.497129	-2.770332	-3.501718
205	6	0	-12.168929	-3.088952	-1.989673
206	1	0	-12.564025	-3.907098	-1.712463

207	6	0	-11.048973	-2.624289	-1.298990
208	6	0	-10.480668	-3.402973	-0.100182
209	6	0	-10.660414	-2.578495	1.185109
210	1	0	-10.210762	-3.030719	1.928310
211	1	0	-11.614521	-2.490935	1.385507
212	1	0	-10.268601	-1.688682	1.059071
213	6	0	-8.992653	-3.734490	-0.308558
214	1	0	-8.882203	-4.228794	-1.147493
215	1	0	-8.672837	-4.283715	0.439583
216	1	0	-8.474025	-2.903918	-0.346783
217	6	0	-11.205409	-4.738061	0.114816
218	1	0	-11.116166	-5.290621	-0.689518
219	1	0	-12.154493	-4.570524	0.292850
220	1	0	-10.806819	-5.206041	0.878954
221	8	0	-3.625696	6.194658	-1.327561
222	1	0	-2.922206	6.625362	-0.688169
223	7	0	-2.384338	7.006900	0.755294
224	6	0	-5.517807	5.276732	1.716619
225	6	0	-5.505214	5.315310	3.129735
226	1	0	-4.782288	5.737173	3.577547
227	6	0	-6.515947	4.753891	3.869384
228	1	0	-6.481875	4.793077	4.817410
229	6	0	-7.596512	4.125783	3.243731
230	1	0	-8.293862	3.739093	3.761576
231	6	0	-7.637035	4.072353	1.884834
232	1	0	-8.370405	3.642486	1.461424
233	6	0	-6.622219	4.639032	1.088722
234	6	0	-6.673527	4.582144	-0.318841
235	1	0	-7.420728	4.168028	-0.735703
236	6	0	-5.697583	5.095973	-1.095988
237	1	0	-5.760255	5.037959	-2.041827
238	6	0	-4.583419	5.718397	-0.495155
239	6	0	-4.474647	5.835121	0.889863
240	6	0	-3.335043	6.508505	1.472287
241	1	0	-3.283348	6.586012	2.417896
242	6	0	-1.251635	7.585820	1.398356
243	6	0	-0.672387	6.896549	2.466735
244	1	0	-1.049859	6.070214	2.747305
245	6	0	0.438164	7.394783	3.123359
246	1	0	0.816252	6.923657	3.855665
247	6	0	0.988959	8.585185	2.697278
248	1	0	1.752216	8.942167	3.136962
249	6	0	0.425009	9.260622	1.624959
250	1	0	0.819229	10.079782	1.348241

251	6	0	-0.694797	8.796793	0.934845
252	6	0	-1.263376	9.574133	-0.263680
253	6	0	-1.084382	8.751177	-1.549332
254	1	0	-1.534156	9.202562	-2.293063
255	1	0	-0.129408	8.662620	-1.750223
256	1	0	-1.475327	7.860361	-1.423785
257	6	0	-2.751217	9.906151	-0.056161
258	1	0	-2.862724	10.400619	0.782720
259	1	0	-3.071130	10.455368	-0.804258
260	1	0	-3.269894	9.075585	-0.017931
261	6	0	-0.539537	10.909862	-0.479555
262	1	0	-0.628736	11.462464	0.324740
263	1	0	0.410445	10.741678	-0.656720
264	1	0	-0.938177	11.377374	-1.242847

Molecular cluster of **25** with five imine tautomers around an enamine form:

E = -5656.12149373 Hartrees

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.443191	-1.267201	-0.939097
2	1	0	0.705227	-0.063523	-0.043319
3	7	0	0.539898	0.200431	0.948015
4	6	0	2.726603	-2.503588	2.307967
5	6	0	2.801831	-2.233381	3.692953
6	1	0	2.340544	-1.341166	4.103097
7	6	0	3.474481	-3.079963	4.561794
8	1	0	3.511469	-2.837523	5.619952
9	6	0	4.108373	-4.237661	4.085883
10	1	0	4.630176	-4.899329	4.769965
11	6	0	4.067248	-4.516616	2.730538
12	1	0	4.554166	-5.405419	2.338578
13	6	0	3.396722	-3.666113	1.828829
14	6	0	3.391087	-3.956332	0.416845
15	1	0	3.935902	-4.834595	0.079288

16	6	0	2.757433	-3.168208	-0.485919
17	1	0	2.767043	-3.387820	-1.548211
18	6	0	2.029968	-1.980481	-0.077079
19	6	0	2.002005	-1.667667	1.352193
20	6	0	1.218854	-0.596411	1.778633
21	1	0	1.122064	-0.365240	2.834655
22	6	0	-0.419443	1.159632	1.347554
23	6	0	-1.197526	0.862064	2.478144
24	1	0	-1.081370	-0.105418	2.954942
25	6	0	-2.148466	1.756333	2.953280
26	1	0	-2.742924	1.505927	3.826487
27	6	0	-2.346740	2.951184	2.269177
28	1	0	-3.103768	3.654293	2.600948
29	6	0	-1.592555	3.231510	1.127573
30	1	0	-1.777873	4.167776	0.619758
31	6	0	-0.605814	2.368360	0.625492
32	6	0	0.217819	2.763428	-0.625285
33	6	0	-0.095606	1.826683	-1.819923
34	1	0	0.434455	2.186690	-2.708569
35	1	0	-1.165367	1.824061	-2.047762
36	1	0	0.218540	0.792359	-1.669786
37	6	0	1.734037	2.732079	-0.315686
38	1	0	1.971305	3.382739	0.531026
39	1	0	2.287630	3.102133	-1.183221
40	1	0	2.104653	1.731324	-0.092381
41	6	0	-0.110177	4.201686	-1.085625
42	1	0	0.099105	4.938593	-0.304233
43	1	0	-1.151962	4.320186	-1.401070
44	1	0	0.520034	4.451560	-1.943646
45	8	0	10.448283	-3.084228	1.739477
46	1	0	9.745912	-3.517769	1.099488
47	7	0	9.210452	-3.903030	-0.343857
48	6	0	12.343995	-2.172712	-1.304508
49	6	0	12.333557	-2.214456	-2.717680
50	1	0	11.611636	-2.637862	-3.165504
51	6	0	13.345071	-1.653150	-3.456591
52	1	0	13.312284	-1.695383	-4.404979
53	6	0	14.424294	-1.022784	-2.830765
54	1	0	15.121780	-0.638168	-3.348095
55	6	0	14.462681	-0.967054	-1.472418
56	1	0	15.195011	-0.535721	-1.048953
57	6	0	13.447097	-1.532698	-0.676493
58	6	0	13.496299	-1.472545	0.730994
59	1	0	14.242532	-1.056945	1.148004

60	6	0	12.519613	-1.985332	1.507962
61	1	0	12.580833	-1.925138	2.453629
62	6	0	11.406786	-2.609973	0.906896
63	6	0	11.300062	-2.729965	-0.478021
64	6	0	10.161830	-3.405525	-1.060719
65	1	0	10.111504	-3.485751	-2.005207
66	6	0	8.079183	-4.483460	-0.986734
67	6	0	7.501156	-3.796808	-2.057708
68	1	0	7.877955	-2.971808	-2.340128
69	6	0	6.392321	-4.298009	-2.715134
70	1	0	6.014100	-3.829398	-3.449182
71	6	0	5.841141	-5.488455	-2.286722
72	1	0	5.079077	-5.846924	-2.726414
73	6	0	6.403733	-6.160205	-1.212782
74	1	0	6.009987	-6.978706	-0.934404
75	6	0	7.522640	-5.693945	-0.521209
76	6	0	8.089563	-6.469298	0.679625
77	6	0	7.907972	-5.643064	1.961286
78	1	0	8.357461	-6.093148	2.707138
79	1	0	6.953254	-5.552054	2.168343
80	1	0	8.298698	-4.752438	1.835320
81	6	0	9.578422	-6.800087	0.474601
82	1	0	9.691554	-7.296405	-0.362814
83	1	0	9.897609	-7.347303	1.224555
84	1	0	10.096512	-5.969258	0.435333
85	6	0	7.366863	-7.804603	0.897100
86	1	0	7.457720	-8.358963	0.094358
87	1	0	6.416440	-7.637167	1.073357
88	1	0	7.764601	-8.270468	1.662972
89	8	0	5.426535	3.976981	1.923577
90	1	0	6.002959	3.333403	1.336791
91	7	0	6.499657	2.778034	-0.064120
92	6	0	4.173524	5.408154	-1.249707
93	6	0	4.282982	5.347408	-2.658825
94	1	0	4.864774	4.709044	-3.053166
95	6	0	3.567367	6.192111	-3.468474
96	1	0	3.662087	6.129667	-4.411251
97	6	0	2.701744	7.143061	-2.923035
98	1	0	2.207373	7.725582	-3.489823
99	6	0	2.573606	7.227010	-1.571014
100	1	0	1.987593	7.875753	-1.201925
101	6	0	3.287433	6.376573	-0.704588
102	6	0	3.147129	6.467679	0.695832
103	1	0	2.542513	7.106010	1.057264

104	6	0	3.842451	5.679750	1.540869
105	1	0	3.727950	5.768513	2.480200
106	6	0	4.741720	4.722947	1.023709
107	6	0	4.914162	4.556768	-0.349558
108	6	0	5.818548	3.544608	-0.848043
109	1	0	5.916088	3.440460	-1.787466
110	6	0	7.433651	1.856275	-0.622289
111	6	0	8.284173	2.307144	-1.634188
112	1	0	8.215544	3.206509	-1.934478
113	6	0	9.224401	1.468631	-2.206812
114	1	0	9.789786	1.782834	-2.902634
115	6	0	9.328435	0.170806	-1.751770
116	1	0	9.968394	-0.418334	-2.134742
117	6	0	8.494399	-0.271471	-0.734697
118	1	0	8.582590	-1.169684	-0.436847
119	6	0	7.532832	0.538125	-0.130685
120	6	0	6.652796	0.001151	1.011300
121	6	0	6.987065	0.743371	2.315627
122	1	0	6.359580	0.471647	3.016707
123	1	0	7.899973	0.523345	2.592798
124	1	0	6.913008	1.710354	2.170373
125	6	0	5.159288	0.161784	0.683932
126	1	0	4.960630	-0.285786	-0.173124
127	1	0	4.618981	-0.241615	1.405724
128	1	0	4.939392	1.115358	0.613759
129	6	0	6.890816	-1.491602	1.268095
130	1	0	6.692988	-1.998480	0.453916
131	1	0	7.826643	-1.635100	1.522104
132	1	0	6.304680	-1.794617	1.993239
133	8	0	-5.591067	-5.953146	-2.187968
134	1	0	-4.888807	-5.520448	-1.548520
135	7	0	-4.353207	-5.134436	-0.104580
136	6	0	-7.486757	-6.864614	0.856042
137	6	0	-7.476437	-6.823722	2.268671
138	1	0	-6.754410	-6.399476	2.717024
139	6	0	-8.487831	-7.384205	3.008096
140	1	0	-8.455157	-7.342819	3.955957
141	6	0	-9.567046	-8.014579	2.382266
142	1	0	-10.264762	-8.400560	2.899918
143	6	0	-9.605432	-8.070305	1.023920
144	1	0	-10.337759	-8.501645	0.600465
145	6	0	-8.589958	-7.505482	0.227489
146	6	0	-8.639158	-7.565642	-1.180000
147	1	0	-9.385387	-7.981254	-1.597030

148	6	0	-7.662471	-7.052851	-1.956954
149	1	0	-7.723575	-7.112227	-2.902116
150	6	0	-6.549532	-6.427360	-1.355371
151	6	0	-6.442955	-6.308190	0.029022
152	6	0	-5.304772	-5.632651	0.611638
153	1	0	-5.254398	-5.552370	1.556215
154	6	0	-3.221720	-4.554270	0.537804
155	6	0	-2.643398	-5.240800	1.608591
156	1	0	-3.021022	-6.065412	1.891473
157	6	0	-1.532710	-4.741075	2.266279
158	1	0	-1.157381	-5.208062	3.000614
159	6	0	-0.982184	-3.552402	1.839657
160	1	0	-0.221585	-3.188214	2.273654
161	6	0	-1.547886	-2.875700	0.765269
162	1	0	-1.153908	-2.055133	0.487954
163	6	0	-2.665649	-3.343568	0.072511
164	6	0	-3.232761	-2.569550	-1.128184
165	6	0	-3.051227	-3.395333	-2.411881
166	1	0	-3.500372	-2.945887	-3.157240
167	1	0	-2.096075	-3.483559	-2.611131
168	1	0	-3.441824	-4.286041	-2.284872
169	6	0	-4.721213	-2.237336	-0.923331
170	1	0	-4.834227	-1.741035	-0.085669
171	1	0	-5.040443	-1.690907	-1.673633
172	1	0	-5.239241	-3.068123	-0.883969
173	6	0	-2.509312	-1.233592	-1.346249
174	1	0	-2.600728	-0.677513	-0.543012
175	1	0	-1.558904	-1.400622	-1.521169
176	1	0	-2.907249	-0.768308	-2.111367
177	8	0	-8.115512	-0.023651	0.974102
178	1	0	-8.818880	-0.457009	0.334084
179	7	0	-9.353426	-0.842456	-1.109308
180	6	0	-6.219837	0.887706	-2.069932
181	6	0	-6.230270	0.846033	-3.483083
182	1	0	-6.952196	0.422684	-3.930893
183	6	0	-5.219714	1.407488	-4.222030
184	1	0	-5.252535	1.365301	-5.170404
185	6	0	-4.140518	2.037864	-3.596181
186	1	0	-3.443052	2.422557	-4.113497
187	6	0	-4.101306	2.093412	-2.237717
188	1	0	-3.369957	2.525063	-1.814299
189	6	0	-5.116846	1.527691	-1.442031
190	6	0	-5.067626	1.587998	-0.034400
191	1	0	-4.321524	2.003873	0.382403

192	6	0	-6.045206	1.075323	0.742516
193	1	0	-5.984002	1.135550	1.688191
194	6	0	-7.158035	0.450676	0.141434
195	6	0	-7.264746	0.330680	-1.243482
196	6	0	-8.402956	-0.344820	-1.826070
197	1	0	-8.452354	-0.425245	-2.770597
198	6	0	-10.485597	-1.422675	-1.752199
199	6	0	-11.062718	-0.736413	-2.822973
200	1	0	-10.685766	0.088654	-3.105380
201	6	0	-12.173088	-1.237696	-3.480680
202	1	0	-12.550407	-0.768598	-4.214507
203	6	0	-12.723653	-2.427593	-3.052640
204	1	0	-13.485905	-2.786105	-3.492569
205	6	0	-12.159758	-3.100341	-1.977869
206	1	0	-12.554587	-3.918055	-1.699393
207	6	0	-11.041138	-2.633203	-1.286624
208	6	0	-10.474000	-3.408716	-0.085206
209	6	0	-10.656251	-2.581421	1.197965
210	1	0	-10.207358	-3.031614	1.942784
211	1	0	-11.610673	-2.494149	1.396721
212	1	0	-10.264927	-1.691655	1.070430
213	6	0	-8.985431	-3.739581	-0.290654
214	1	0	-8.873395	-4.235699	-1.128271
215	1	0	-8.666308	-4.286828	0.459171
216	1	0	-8.467407	-2.908733	-0.330015
217	6	0	-11.198061	-4.743875	0.131776
218	1	0	-11.107227	-5.298168	-0.671130
219	1	0	-12.147483	-4.576631	0.308027
220	1	0	-10.800262	-5.209790	0.897531
221	8	0	-3.624416	6.191209	-1.324403
222	1	0	-2.922107	6.623972	-0.685034
223	7	0	-2.387263	7.009170	0.758135
224	6	0	-5.520482	5.278737	1.719146
225	6	0	-5.509723	5.320971	3.131903
226	1	0	-4.787932	5.743964	3.580010
227	6	0	-6.521240	4.760177	3.871597
228	1	0	-6.488514	4.801487	4.819426
229	6	0	-7.600439	4.129802	3.245744
230	1	0	-8.298156	3.743828	3.763374
231	6	0	-7.638929	4.073286	1.886859
232	1	0	-8.371239	3.641899	1.463395
233	6	0	-6.623274	4.638948	1.090821
234	6	0	-6.672562	4.578698	-0.316573
235	1	0	-7.418730	4.163112	-0.733524

236	6	0	-5.695871	5.091538	-1.093528
237	1	0	-5.757177	5.031253	-2.039234
238	6	0	-4.582851	5.716272	-0.492373
239	6	0	-4.476319	5.836033	0.892676
240	6	0	-3.337930	6.511626	1.475075
241	1	0	-3.287886	6.591383	2.420513
242	6	0	-1.255222	7.590557	1.401606
243	6	0	-0.676972	6.904001	2.472501
244	1	0	-1.054788	6.077953	2.754100
245	6	0	0.431979	7.404358	3.129848
246	1	0	0.809349	6.935505	3.863476
247	6	0	0.982531	8.594482	2.701638
248	1	0	1.744827	8.953017	3.141561
249	6	0	0.419677	9.267058	1.626910
250	1	0	0.813617	10.085792	1.348912
251	6	0	-0.698783	8.800714	0.936256
252	6	0	-1.266208	9.574912	-0.264902
253	6	0	-1.084717	8.749152	-1.548435
254	1	0	-1.533735	9.198506	-2.293784
255	1	0	-0.129432	8.660883	-1.747681
256	1	0	-1.475176	7.858385	-1.421390
257	6	0	-2.754658	9.906304	-0.060303
258	1	0	-2.867718	10.402577	0.777249
259	1	0	-3.073833	10.453547	-0.810094
260	1	0	-3.272708	9.075461	-0.020940
261	6	0	-0.543052	10.910745	-0.482768
262	1	0	-0.633858	11.465058	0.320112
263	1	0	0.407259	10.742843	-0.658145
264	1	0	-0.940934	11.376157	-1.247667