

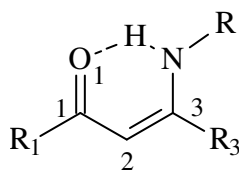
Interplay between steric and electronic factors in determining the strength of intramolecular N-H...O resonance-assisted hydrogen bonds (RAHBs) in β -enaminones.

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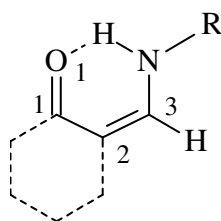
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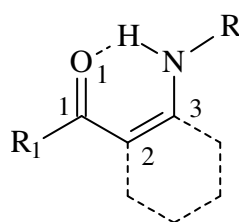
**Supplementary Tables
S1-S6**

Table S1. Structural data (Å, °) for β -enaminones of sub-Class **Ia**.**Ia**

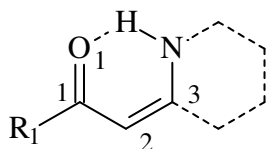
REFCODE	O...N	O1=C1	C1-C2	C2=C3	C3-N	O1=C1-C2	C1-C2=C3	C2=C3-N
BAKBEU	2.668	1.255	1.419	1.386	1.334	123.6	123.5	121.3
BEQXOK	2.637	1.264	1.407	1.381	1.330	122.7	123.9	120.8
CAVDUY	2.686	1.256	1.399	1.377	1.339	122.9	125.5	121.0
CIMCAC	2.653	1.245	1.426	1.374	1.343	125.1	122.6	121.0
DAXYIK	2.687	1.238	1.402	1.393	1.331	125.6	122.8	121.6
EHUNIE	2.648	1.236	1.424	1.349	1.336	124.0	122.8	122.5
	2.670	1.245	1.395	1.398	1.310	123.0	124.5	121.2
EHUNOK	2.658	1.274	1.413	1.385	1.335	122.4	124.1	121.4
EHUNUQ	2.640	1.264	1.408	1.400	1.318	123.0	122.7	121.8
	2.631	1.247	1.440	1.372	1.320	122.3	122.9	121.9
ETACIM	2.725	1.243	1.440	1.392	1.335	124.5	124.0	121.3
	2.725	1.246	1.441	1.395	1.329	124.0	124.6	120.7
FAGQEJ	2.635	1.249	1.415	1.369	1.342	123.1	123.4	121.0
	2.653	1.249	1.415	1.369	1.339	122.7	123.9	121.9
GEMYEC	2.653	1.280	1.400	1.398	1.326	122.2	123.4	122.4
GEZSEJ	2.695	1.245	1.407	1.370	1.335	124.7	124.9	120.7
HOKXUA	2.638	1.254	1.415	1.358	1.364	123.4	124.5	120.2
	2.672	1.244	1.430	1.371	1.355	124.8	123.1	121.2
HUHXIR	2.637	1.241	1.414	1.373	1.335	123.2	124.6	119.6
	2.643	1.245	1.415	1.368	1.339	123.4	124.8	119.5
IPAMOB	2.653	1.246	1.421	1.361	1.335	122.9	125.1	119.8
	2.679	1.244	1.418	1.368	1.357	123.5	124.7	120.9
IPAMUH	2.679	1.242	1.406	1.375	1.332	122.4	124.9	121.9
JADSUC	2.677	1.269	1.404	1.393	1.328	121.6	124.7	122.3
KONWIT	2.654	1.253	1.435	1.364	1.346	121.5	123.3	122.9
KUXJUI	2.668	1.266	1.405	1.381	1.341	122.2	125.2	120.9
	2.681	1.267	1.405	1.381	1.339	121.9	125.2	121.7
KUXJUI01	2.662	1.272	1.406	1.376	1.339	122.1	124.4	122.0
MAMTEZ	2.673	1.245	1.376	1.393	1.355	124.4	124.6	129.7
	2.700	1.264	1.382	1.391	1.341	124.9	125.5	120.0
NERBUH	2.663	1.255	1.407	1.384	1.338	123.0	125.4	119.6
	2.659	1.246	1.417	1.380	1.340	123.0	124.6	120.2
	2.656	1.248	1.419	1.369	1.335	122.9	124.2	121.3
	2.658	1.249	1.427	1.373	1.336	121.8	124.9	120.8
OKAHUD	2.634	1.260	1.409	1.382	1.336	122.0	124.3	120.8
OPAMPR	2.669	1.245	1.434	1.376	1.332	122.7	123.9	121.7
PESNUW	2.652	1.259	1.416	1.375	1.345	123.0	124.7	120.1
PICFOW	2.660	1.245	1.429	1.352	1.362	122.8	125.7	119.6
PICGEN	2.681	1.252	1.401	1.384	1.333	122.8	125.3	120.9
TICLIA	2.712	1.250	1.398	1.374	1.350	123.6	125.1	122.1
VUBJUX	2.676	1.257	1.404	1.396	1.314	123.2	123.8	122.0
XUKFAK	2.684	1.240	1.427	1.374	1.349	121.9	125.7	120.6
YIJSAL	2.702	1.243	1.420	1.357	1.352	122.9	125.7	121.4
ZIZVIN	2.701	1.249	1.426	1.356	1.370	122.5	124.7	122.7
RALROM	2.628	1.264	1.419	1.385	1.339	121.9	124.5	120.7
GAVWIK	2.670	1.250	1.431	1.370	1.356	122.9	124.1	121.2
	<2.67[2]>	<1.25[1]>	<1.41[1]>	<1.38[1]>	<1.34[1]>	<123[1]>	<124.4[9]>	<121.1[9]>

Table S2. Structural data (Å, °) for β -enaminones of sub-Classes **Ib** and **Ic**.**Ib**

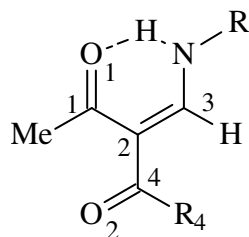
REFCODE	O...N	O1=C1	C1-C2	C2=C3	C3-N	O1=C1-C2	C1-C2=C3	C2=C3-N
CABVUW	2.650	1.255	1.414	1.378	1.353	122.4	121.5	125.3
	2.649	1.257	1.421	1.345	1.354	122.5	121.7	125.7
	<2.650>	<1.256>	<1.418>	<1.362>	<1.354>	<122.4>	<121.6>	<125.5>

**Ic**

REFCODE	O...N	O1=C1	C1-C2	C2=C3	C3-N	O1=C1-C2	C1-C2=C3	C2=C3-N
YAPDEY	2.602	1.258	1.427	1.393	1.346	123.8	121.0	121.2
XACHUE	2.573	1.263	1.426	1.390	1.340	123.3	120.3	121.4
YARYOG	2.598	1.244	1.433	1.387	1.345	123.8	120.2	122.5
	2.614	1.237	1.437	1.374	1.346	124.0	120.5	122.6
DAPCED	2.576	1.249	1.435	1.383	1.349	123.5	120.6	121.5
	<2.59[2]>	<1.25[1]>	<1.432[5]>	<1.385[7]>	<1.345[3]>	<123.7[3]>	<120.5[3]>	<121.8[6]>

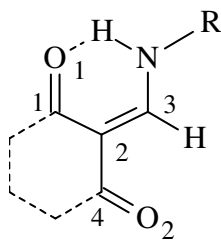
Table S3. Structural data (Å, °) for β -enaminones of sub-Class **Id**.**Id**

REFCODE	O...N	O1=C1	C1-C2	C2=C3	C3-N	O1=C1-C2	C1-C2=C3	C2=C3-N
KOKBIV01	2.605	1.250	1.431	1.371	1.349	122.4	123.0	120.5
LOBHEP	2.600	1.272	1.403	1.399	1.354	122.9	122.9	119.9
LOBHEP02	2.600	1.270	1.411	1.398	1.356	123.1	122.5	120.0
LOBHIT	2.582	1.275	1.400	1.404	1.363	122.5	122.7	119.8
LOBHOZ	2.588	1.260	1.406	1.397	1.352	123.2	121.8	120.8
LOGBUE	2.622	1.268	1.410	1.391	1.361	122.5	123.4	120.5
	2.575	1.282	1.402	1.396	1.362	122.1	123.0	119.7
QAPKOH	2.590	1.279	1.396	1.392	1.345	122.1	123.4	120.2
QIGGUI	2.620	1.246	1.432	1.382	1.345	121.5	122.9	121.9
	2.609	1.239	1.425	1.391	1.336	122.4	122.4	121.1
	2.608	1.250	1.405	1.374	1.351	122.9	123.0	121.3
	2.611	1.258	1.423	1.365	1.350	122.0	122.9	121.6
CAPKEK	2.617	1.251	1.431	1.395	1.334	123.6	121.4	121.6
CAPKIO	2.638	1.245	1.423	1.406	1.326	123.9	121.5	122.2
	2.616	1.252	1.421	1.401	1.330	122.5	122.2	121.6
CAPKOU	2.637	1.254	1.433	1.402	1.335	123.2	121.6	122.2
	2.629	1.257	1.434	1.397	1.332	123.2	121.4	122.4
	<2.61[2]>	<1.26[1]>	<1.42[1]>	<1.39[1]>	<1.35[1]>	<122.7[6]>	<122.5[7]>	<121.0[8]>

Table S4. Structural data (Å, °) for β - β' -diketoenamines of sub-Class **IIa**.**IIa**

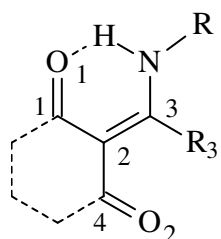
REFCODE	O...N	O1=C1	C1-C2	C2=C3	C3-N	O1=C1-C2	C1-C2=C3	C2=C3-N
AKEWUI	2.617	1.242	1.462	1.387	1.330	120.7	119.6	125.6
BIPLIV	2.593	1.237	1.460	1.390	1.324	120.7	119.0	125.8
CAGKAX	2.610	1.249	1.449	1.380	1.329	120.0	120.1	126.6
	2.610	1.238	1.449	1.388	1.330	121.5	119.4	125.7
COVJUS	2.572	1.249	1.439	1.413	1.308	119.7	120.1	124.1
GIVCOD	2.580	1.243	1.452	1.400	1.318	120.9	119.3	124.8
POVCEI	2.638	1.247	1.453	1.387	1.320	120.2	119.6	128.1
CAGJOK	2.559	1.242	1.454	1.387	1.331	120.5	119.9	123.9
	2.588	1.237	1.453	1.386	1.323	120.8	120.2	124.6
CAGJUQ	2.576	1.238	1.465	1.379	1.326	120.0	119.4	125.8
FEVBOY	2.652	1.236	1.445	1.389	1.300	120.0	120.3	127.7
NIHNAT	2.625	1.241	1.445	1.384	1.315	120.7	119.7	127.5
	2.592	1.247	1.429	1.395	1.307	121.2	120.1	125.1
	2.656	1.239	1.438	1.406	1.306	120.6	120.7	126.9
	2.651	1.235	1.454	1.392	1.323	120.9	119.5	126.6
RUXLAX	2.619	1.236	1.447	1.395	1.310	121.2	120.3	125.4
CANDAX	2.630	1.234	1.451	1.388	1.301	120.9	119.1	127.8
	<2.61[3]>	<1.240[5]>	<1.450[9]>	<1.390[9]>	<1.32[1]>	<120.5[5]>	<119.8[4]>	<126[1]>

Table S5. Structural data (Å, °) for β - β' -diketoenamines of sub-Classes **IIb** and **IIc**.



IIb

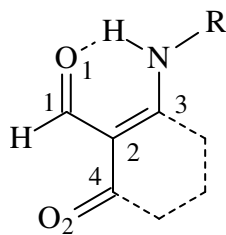
REFCODE	O...N	O1=C1	C1-C2	C2=C3	C3-N	O1=C1C2	C1-C2=C3	C2=C3-N
GAFTOW	2.647	1.262	1.437	1.409	1.315	120.7	122.3	123.3
ISUQAO	2.640	1.234	1.438	1.391	1.311	121.9	121.5	124.0
KOHPAY	2.606	1.237	1.410	1.391	1.360	123.1	122.6	120.7
	<2.63[2]>	<1.24[2]>	<1.43[2]>	<1.40[1]>	<1.33[3]>	<122[2]>	<122.1[6]>	<123[2]>



IIc

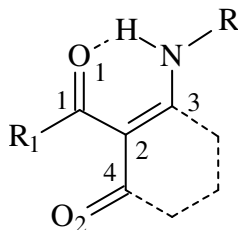
GOWYOG01	2.532	1.265	1.438	1.423	1.319	123.4	121.0	117.0
GOXLOU01	2.536	1.251	1.448	1.419	1.320	123.1	120.5	118.1
GOXRIU	2.563	1.258	1.446	1.438	1.303	123.5	120.4	118.6
PAEXPY02	2.526	1.262	1.445	1.427	1.322	123.5	120.7	117.0
WIXKAP	2.558	1.263	1.448	1.406	1.312	122.6	120.1	119.1
ZECZUC	2.553	1.255	1.427	1.433	1.307	124.2	121.3	117.9
LARRAY	2.540	1.262	1.442	1.437	1.312	123.5	120.7	117.4
	2.560	1.257	1.447	1.430	1.312	123.9	120.7	118.1
LARREC	2.540	1.254	1.445	1.426	1.322	123.6	120.4	118.1
	2.561	1.247	1.437	1.416	1.323	123.7	120.4	119.6
XACMUK	2.570	1.255	1.441	1.441	1.309	123.8	120.6	118.6
	2.578	1.251	1.440	1.436	1.314	123.9	120.9	118.1
HABNED	2.544	1.263	1.446	1.438	1.311	123.4	120.2	118.4
IXAZIQ	2.561	1.253	1.430	1.438	1.308	123.7	120.8	118.6
	<2.55[2]>	<1.257[5]>	<1.442[6]>	<1.428[9]>	<1.315[6]>	<123.6[4]>	<120.6[3]>	<118.1[7]>

Table S6. Structural data (Å, °) for β - β' -diketoenamines of sub-Classes **II**d and **II**e.



IId

REFCODE	O...N	O1=C1	C1-C2	C2=C3	C3-N	O1=C1-C2	C1-C2=C3	C2=C3-N
YITCIN	2.644	1.244	1.426	1.409	1.350	125.9	122.6	118.4



IIe

RENRIX	2.573	1.231	1.458	1.411	1.337	121.5	119.8	122.0
RENSAE	2.594	1.248	1.443	1.412	1.319	121.9	120.5	121.9
	<2.584>	<1.240>	<1.450>	<1.412>	<1.328>	<121.7>	<120.2>	<122.0>