Supplementary Material (ESI) for New Journal of Chemistry

Substituent effects on keto-enol tautomerization of β-diketones from X-ray structural data and DFT calculations.

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Supplementary Data

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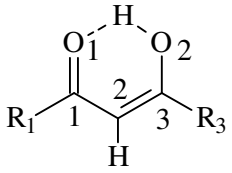
Table S1. REFCODEs and intramolecular O…O H-bond distances (Å) for β-keto-enols of Class **I.** (**1a-1j**) refer to the structures of acetylacetone or compounds forming co-crystals containing molecules of acetylacetone).



R_1,R_3 = any substituent linked by a Carbon atom

Structure	REFCODE	$d_{O...O}$
1a	LIWPIQ	2.541
1b	LIWPIQ01	2.547
1c	ACAGAN	2.507; 2.536
1d	DPHEAD10	2.535
1e	DPHEAD20	2.536
1f	HADJUS	2.509
1g	HADKAZ	2.517; 2.528
1h	IBOWAX	2.474
1i	QASGAS	2.488; 2.515
1j	TITZEB	2.493
2	AGIFAX	2.501; 2.478
3	AHEQOT	2.498
4a	APUSAF	2.464
4b	APUSAF01	2.444
5	AVABEE	2.488
6	BEMCAX	2.516
7	BILWEZ	2.516
8	BILWID	2.534
9a	BINMEQ	2.447
9b	BINMEQ01	2.454
10	BOLZAD	2.485
11	BOLZEH	2.495
12	BPBUDO	2.482
13	BUWKUZ	2.514
14a	BZOYAC	2.497
14b	BZOYAC01	2.485
14c	BZOYAC02	2.493
14d	BZOYAC03	2.500
14e	BZOYAC04	2.502
14f	BZOYAC05	2.499
14g	BZOYAC06	2.501
15a	CACBAK	2.509
15b	CACBAK01	2.495; 2.505
16	CEBMOL	2.511

17	CESMIW	2.485
18	DAMTAM	2.495
19a	DBEZLM	2.460
19b	DBEZLM01	2.461
19c	DBEZLM02	2.459
19d	DBEZLM03	2.452
19e	DBEZLM04	2.461
19f	DBEZLM05	2.459
20	DEBFEV	2.561; 2.565
21	DEJYOH	2.488
22	DUKRUW	2.557; 2.562
23	EMUPAD	2.562
24a	EVEXAE	2.434
24b	EVEXAE01	2.439
24c	EVEXAE01	2.448
25	EYIZER	2.541
26	EYIZIV	2.472
27	FAXWAD	2.436
28	FIPXEH	2.518; 2.526
29	FIZWER	2.504
30a	FOLHAP	2.496
30b	FOHLAP01	2.493
31	FULCEU	2.553
32	GANJAG	2.508
33	HANHOU	2.500
34	HECGIF	2.536
35	HUZGAK	2.498
36	JERWIN	2.471; 2.526
37	JITVUD	2.465
38	JITWAX	2.470
39	JITWEO	2.461
40	JITWIS	2.502
41	JITWOY	2.492
42a	JITWUE	2.554
42b	JITWUE01	2.558
42c	JITWUE02	2.559
42d	JITWUE03	2.558
42e	JITWUE04	2.556
43	JITXAL	2.432, 2.434
44	JITXEP	2.499
45	JUDBIT	2.461
46	JUJTIR	2.541
47	KASPOK	2.459
48	KATJIZ	2.495
49	KAWXEL	2.516
50	KAZKIF	2.490
51	KEHZEC	2.514; 2.517
52	KEMQUO	2.452
53	KIQLUR	2.551
54a	KOJYEN	2.487
54b	KOJYEN02	2.473

55	KOJYIR	2.539
56	KUGRIN	2.471
57	LEPLIC	2.543
58	LEPLOI	2.509; 2.512
59	LEPLUO	2.552
60	LIKBAI	2.509
61	LUQLEO	2.464
62	LUQLOY	2.452
63	NAMFUD	2.512
64	NENLOI	2.444
65	NPBUDO	2.459
66	OKEREB	2.534
67	QEMREF	2.546
68	RIMFUO	2.519; 2.523
69	SARHUP	2.481
70	SEBVOL	2.525; 2.539; 2.541; 2.555
71	TALJEV	2.540
72	THTFBD	2.522; 2.551
73	TOLACP10	2.455
74	TUBYOE	2.459
75	UGOLEH	2.524
76	VIDREF	2.535
77	VOKQAN	2.479
78	WEBGAL	2.473
79a	WIDCER	2.531; 2.535
79b	WIDCER01	2.533
80	WIDCIV	2.449
81	XEDHAQ	2.506
82	XEGXEM	2.462
83	XEPJIL	2.538
84	XEPJOR	2.511
85	XEYRUO	2.559
86	XEYSEZ	2.491; 2.514
87	YAVROC	2.515; 2.530
88	YEBQUS	2.548
89	Bouhaine et al. Acta Cryst. (2006) E62, o5401	2.456
90	Wang et al. Acta Cryst. (2007) E63, o296	2.490
91	Zheng et al. Acta Cryst. (2007) E63, o396	2.486
92	Parimita et al. Acta Cryst. (2007)) E63, o860	2.455
93	Zheng et al. Acta Cryst. (2007) E63, o966	2.503, 2.518