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*Supporting Information Available:*

| $d$(Å) | K17 | K19 | E9c | E9t | K37 | E7c |
|---|---|---|---|---|---|---|
| N1-C2 | 1.385 | 1.373 | 1.358 | 1.357 | 1.308 | 1.366 |
| C2-N3 | 1.311 | 1.318 | 1.346 | 1.351 | 1.384 | 1.339 |
| N3-C4 | 1.379 | 1.369 | 1.348 | 1.346 | 1.383 | 1.356 |
| C4-C5 | 1.411 | 1.411 | 1.420 | 1.414 | 1.395 | 1.424 |
| C5-C6 | 1.439 | 1.454 | 1.414 | 1.414 | 1.457 | 1.403 |
| C6-N1 | 1.428 | 1.448 | 1.345 | 1.339 | 1.425 | 1.336 |
| C5-N7 | 1.382 | 1.386 | 1.393 | 1.393 | 1.388 | 1.387 |
| N7-C8 | 1.380 | 1.326 | 1.324 | 1.326 | 1.374 | 1.385 |
| C8-N9 | 1.331 | 1.389 | 1.391 | 1.390 | 1.341 | 1.326 |
| N9-C4 | 1.383 | 1.383 | 1.385 | 1.389 | 1.371 | 1.390 |
| C6-O10 | 1.241 | 1.233 | 1.353 | 1.358 | 1.242 | 1.364 |
| C2-H | 1.097 | 1.096 | 1.097 | 1.097 | 1.099 | 1.097 |
| C8-H | 1.091 | 1.091 | 1.092 | 1.092 | 1.091 | 1.092 |
| H- | N1<br>1.025 | N1<br>1.025 | O10<br>0.987 | O10<br>0.985 | N3<br>1.022 | O10<br>0.987 |
| H- | N7<br>1.022 | N9<br>1.022 | N9<br>1.021 | N9<br>1.021 | N7<br>1.022 | N7<br>1.027 |

Interatomic distances (Å) for the six most stable hypoxanthine tautomers.

| Angle | K17 | K19 | E9c | E9t | K37 | E7c |
|---|---|---|---|---|---|---|
| C2-N1-C6 | 125.49 | 126.75 | 118.46 | 117.75 | 120.95 | 117.63 |
| N1-C2-N3 | 125.45 | 124.53 | 128.07 | 128.94 | 126.61 | 128.46 |
| C2-N3-C4 | 113.51 | 111.69 | 111.34 | 111.09 | 117.03 | 113.36 |
| N3-C4-C5 | 123.94 | 129.32 | 127.52 | 126.63 | 118.38 | 122.99 |
| C4-C5-C6 | 123.54 | 118.91 | 114.29 | 115.55 | 124.08 | 117.96 |
| N1-C6-C5 | 108.07 | 108.81 | 120.32 | 120.04 | 112.95 | 119.59 |
| N1-C6-O10 | 122.29 | 119.99 | 118.27 | 117.50 | 122.80 | 119.49 |
| C5-C6-O10 | 129.64 | 131.20 | 121.41 | 122.46 | 124.25 | 120.93 |
| N3-C4-N9 | 125.58 | 125.86 | 128.03 | 129.17 | 128.55 | 126.86 |
| C5-C4-N9 | 110.49 | 104.83 | 104.45 | 104.20 | 113.07 | 110.15 |
| C4-C5-N7 | 105.55 | 111.10 | 111.35 | 111.80 | 103.73 | 105.54 |
| C6-C5-N7 | 130.90 | 129.99 | 134.36 | 132.65 | 132.19 | 136.49 |
| C5-N7-C8 | 106.21 | 104.38 | 103.83 | 103.67 | 107.13 | 105.84 |
| C4-N9-C8 | 104.43 | 106.67 | 106.64 | 106.83 | 103.13 | 104.44 |
| N7-C8-N9 | 113.32 | 113.02 | 113.73 | 113.51 | 112.93 | 114.03 |
| N1-C2-H | 115.16 | 116.21 | 115.60 | 115.26 | 119.14 | 114.97 |
| N3-C2-H | 119.38 | 119.26 | 116.34 | 115.80 | 114.25 | 116.57 |
| N7-C8-H | 121.71 | 125.27 | 124.87 | 125.00 | 122.48 | 121.16 |
| N9-C8-H | 124.96 | 121.72 | 121.40 | 121.50 | 124.59 | 124.81 |
| H | N1 – C2 119.50 | N1 – C2 119.33 | O10 – C6 104.99 | O10 – C6 106.90 | N3 – C2 121.90 | O10 – C6 105.18 |
| H | N1 – C6 115.01 | N1 – C6 113.92 | – | – | N3 – C4 121.07 | — |
| H | N7 – C5 125.74 | N9 – C4 125.53 | N9 – C4 125.73 | N9 – C4 125.94 | N7 – C5 124.69 | N7 – C5 126.97 |
| H | N7 – C8 128.05 | N9 – C8 127.80 | N9 – C8 127.64 | N9 – C8 127.23 | N7 – C8 128.18 | N7 – C8 127.19 |

Angles (degrees) for the six most stable hypoxanthine tautomers.

| cis-N(9)-H enolic tautomer | | | trans-N(9)-H enolic tautomer | | |
|---|---|---|---|---|---|
| $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments | $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments |
| 3533.95 | 74.20 | $\nu$ OH | 3566.66 | 65.61 | $\nu$ OH |
| 3510.96 | 80.75 | $\nu$ N(9)-H | 3510.49 | 81.26 | $\nu$ N(9)-H |
| 3160.87 | 0.94 | $\nu$ C(8)-H | 3163.89 | 0.56 | $\nu$ C(8)-H |
| 3097.44 | 18.09 | $\nu$ C(2)-H | 3096.94 | 19.02 | $\nu$ C(2)-H |
| 1608.88 | 137.45 | Rings vib.<br>$\delta$ COH*<br>N(9) – H vib. | 1598.19 | 131.88 | Rings vib.<br>$\delta$ COH*<br>N(9) – H vib. |
| 1564.79 | 198.93 | Rings vib.<br>$\nu$ C – O<br>N(9) – H/C(2) – H vib. | 1567.81 | 333.92 | Rings vib.<br>C(2) – H vib.<br>$\delta$ COH*<br>N(9) – H vib. |
| 1462.54 | 21.66 | Rings vib.<br>C(8) – H vib.<br>$\delta$ COH* | 1465.46 | 46.17 | Rings vib.<br>C(2) – H/C(8) – H vib.<br>$\delta$ COH*<br>N(9) – H vib. |
| 1446.78 | 141.67 | Rings vib.<br>$\delta$ COH*<br>C(2) – H vib. | 1457.33 | 11.85 | Rings vib.<br>C(2) – H/C(8) – H vib.<br>$\nu$ C – O |
| 1389.03 | 38.49 | Rings vib.<br>$\delta$ COH* | 1378.72 | 75.17 | Rings vib.<br>$\delta$ COH* |
| 1365.26 | 7.66 | C(2) – H/N(9) – H vib.<br>Rings vib.<br>$\nu$ C – O | 1369.40 | 0.44 | Rings vib.<br>C(2) – H vib.<br>N(9) – H vib.<br>$\delta$ COH* |
| 1327.64 | 136.21 | Rings vib.<br>N(9) – H vib.<br>$\delta$ COH* | 1336.47 | 23.34 | Rings vib.<br>N(9) – H vib.<br>$\delta$ COH* |
| 1309.95 | 85.27 | Rings vib.<br>C(8) – H vib.<br>$\delta$ COH* | 1313.28 | 20.39 | Rings vib.<br>$\delta$ COH*<br>C(8) – H vib. |

Vibrational modes analysis for the N(9)-H enolic tautomers.

$\delta$ COH* means $\nu$ and $\delta$ combined modes for this group.

| cis-N(9)-H enolic tautomer | | | trans-N(9)-H enolic tautomer | | |
|---|---|---|---|---|---|
| $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments | $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments |
| 1296.65 | 12.64 | Rings vib. C(2) – H vib. N(9) – H vib. $\delta$ COH* | 1292.27 | 67.04 | Rings vib. C(2) – H/N(9) – H /C(8) – H vib. $\delta$ COH |
| 1264.27 | 17.75 | Rings vib. $\delta$ COH* N(9) – H vib. | 1266.70 | 216.37 | Rings vib. $\delta$ COH* |
| 1218.05 | 22.29 | Rings vib. C(8) – H vib. N(9) – H vib. $\nu$ C – O | 1215.99 | 15.72 | Rings vib. C(8) – H/N(9) – H vib. $\nu$ C – O |
| 1106.41 | 5.26 | Rings vib. C(8) – H vib. $\delta$ COH* | 1114.58 | 49.17 | Rings vib. C(8) – H vib. $\delta$ COH* |
| 1060.47 | 176.47 | Rings vib. $\delta$ COH* C(8) – H vib. | 1073.91 | 21.35 | Rings vib. $\delta$ COH* C(8) – H vib. |
| 1037.85 | 10.08 | Rings vib. N(9) – H vib. | 1043.07 | 16.43 | Rings vib. N(9) – H vib. $\delta$ COH |
| 911.04 | 8.52 | C(2)-H vib.[a] | 916.12 | 6.51 | C(2) – H vib.[a] Pirimidinic ring vib. |
| 899.27 | 15.61 | Rings vib. $\nu$ C – O C(2) – H vib. | 900.51 | 14.43 | Rings vib. $\nu$ C – O |
| 857.16 | 13.69 | Rings vib. $\nu$ C – O | 850.04 | 17.43 | Rings vib. $\nu$ C – O |
| 798.63 | 10.50 | C(8) – H vib.[a] Rings vib. | 794.36 | 10.19 | C(8) – H vib.[a] Rings vib. |
| 762.47 | 17.04 | C(8) – H vib.[a] Rings vib. | 763.18 | 15.84 | C(8) – H vib.[a] Rings vib. |
| 698.50 | 1.83 | Rings vib. $\delta$ COH* | 702.56 | 2.15 | Rings vib. $\nu$ C – O |

Vibrational modes analysis for the N(9)-H enolic tautomers (Continuation).

| cis-N(9)-H enolic tautomer | | | trans-N(9)-H enolic tautomer | | |
|---|---|---|---|---|---|
| $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments | $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments |
| 656.62 | 21.31 | Rings vib.[a] $\delta$ COH* | 648.69 | 4.49 | Rings vib.[a] $\nu$ C − O C(8) − H vib. |
| 639.18 | 6.35 | Rings vib.[a] $\delta$ OH | 635.10 | 1.71 | Rings vib.[a] |
| 590.06 | 1.36 | Rings vib. | 603.52 | 9.70 | Rings vib. |
| 555.77 | 15.00 | Rings vib.[a] N(9) − H vib. OH vib. | 552.65 | 47.85 | Rings vib.[a] N(9) − H vib. |
| 550.58 | 118.61 | OH vib.[a] Rings vib. | 536.63 | 110.13 | O-H vib.[a] |
| 510.21 | 8.49 | Rings vib. | 518.71 | 17.26 | Pirimidinic ring vib. |
| 506.53 | 0.79 | Rings vib. | 507.61 | 0.41 | Pirimidinic ring vib. |
| 482.84 | 59.87 | N(9) − H vib.[a] Rings vib. $\delta$ OH | 487.53 | 73.18 | N(9) − H vib.[a] Rings vib. |
| 287.95 | 12.60 | Rings vib. $\nu$ COH | 286.53 | 0.49 | Rings vib.[a] |
| 284.43 | 0.45 | Rings vib.[a] | 269.16 | 7.53 | Pirimidinic ring vib. |
| 207.89 | 14.10 | Rings vib.[a] OH vib. | 205.95 | 1.53 | Rings vib.[a] $\delta$ OH |
| 154.44 | 2.96 | Rings vib.[a] $\delta$ COH* | 157.82 | 3.01 | Rings vib.[a] $\delta$ COH* |

Vibrational modes analysis for the N(9)-H enolic tautomers (Continuation).

| N(3)-H/N(7)-H ketonic tautomer | | | cis-N(7)-H enolic tautomer | | |
|---|---|---|---|---|---|
| $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments | $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments |
| 3507.39 | 93.10 | $\nu$ N(7)-H | 3539.33 | 73.74 | $\nu$ OH |
| 3486.52 | 76.92 | $\nu$ N(3)-H | 3514.50 | 75.52 | $\nu$ N(7)-H |
| 3176.36 | 1.46 | $\nu$ C(8)-H | 3159.87 | 1.79 | $\nu$ C(8)-H |
| 3071.50 | 21.16 | $\nu$ C(2)-H | 3095.04 | 21.27 | $\nu$ C(2)-H |
| 1665.85 | 551.26 | $\nu$ C = O<br>Pirimidinic ring vib. | 1636.47 | 137.29 | Rings vib.<br>$\delta$ COH* |
| 1594.62 | 87.97 | Pirimidinic ring vib.<br>$\nu$ C = O | 1532.92 | 231.41 | Rings vib.<br>$\delta$ COH* |
| 1543.23 | 62.56 | Rings vib.<br>N(3) – H vib.<br>N(7) – H vib.<br>$\nu$ C = O | 1468.34 | 55.48 | Rings vib.<br>C(8) – H/N(7) – H vib.<br>$\delta$ COH<br>C(2) – H vib. |
| 1500.05 | 85.81 | Rings vib.<br>C(2) – H vib. | 1453.02 | 15.21 | Rings vib.<br>C(2) – H vib.<br>$\nu$ C – O |
| 1422.43 | 50.39 | Rings vib.<br>C(8) – H vib.<br>N(3) – H vib. | 1368.29 | 86.33 | Rings vib.<br>N(7) – H vib.<br>$\delta$ COH*<br>C(2) – H vib. |
| 1399.32 | 82.81 | Rings vib.<br>N(7) – H/N(3) – H vib. | 1355.28 | 143.05 | Rings vib.<br>C(8) – H vib.<br>$\delta$ COH* |
| 1358.65 | 23.92 | Rings vib.<br>C(2) – H vib. | 1338.38 | 54.50 | Rings vib.<br>C(2) – H/C(8) – H vib.<br>$\nu$ C – O |
| 1328.31 | 11.64 | Rings vib.<br>N(7) – H/N(3) – H vib. | 1318.74 | 36.00 | Rings vib.<br>C(2) – H vib.<br>$\delta$ COH*<br>N(7) – H/C(8) – H vib. |
| 1299.82 | 7.34 | Rings vib.<br>C(2) – H/N(3) – H vib. | 1284.26 | 2.23 | Rings vib.<br>$\delta$ COH*<br>C – H vib. |

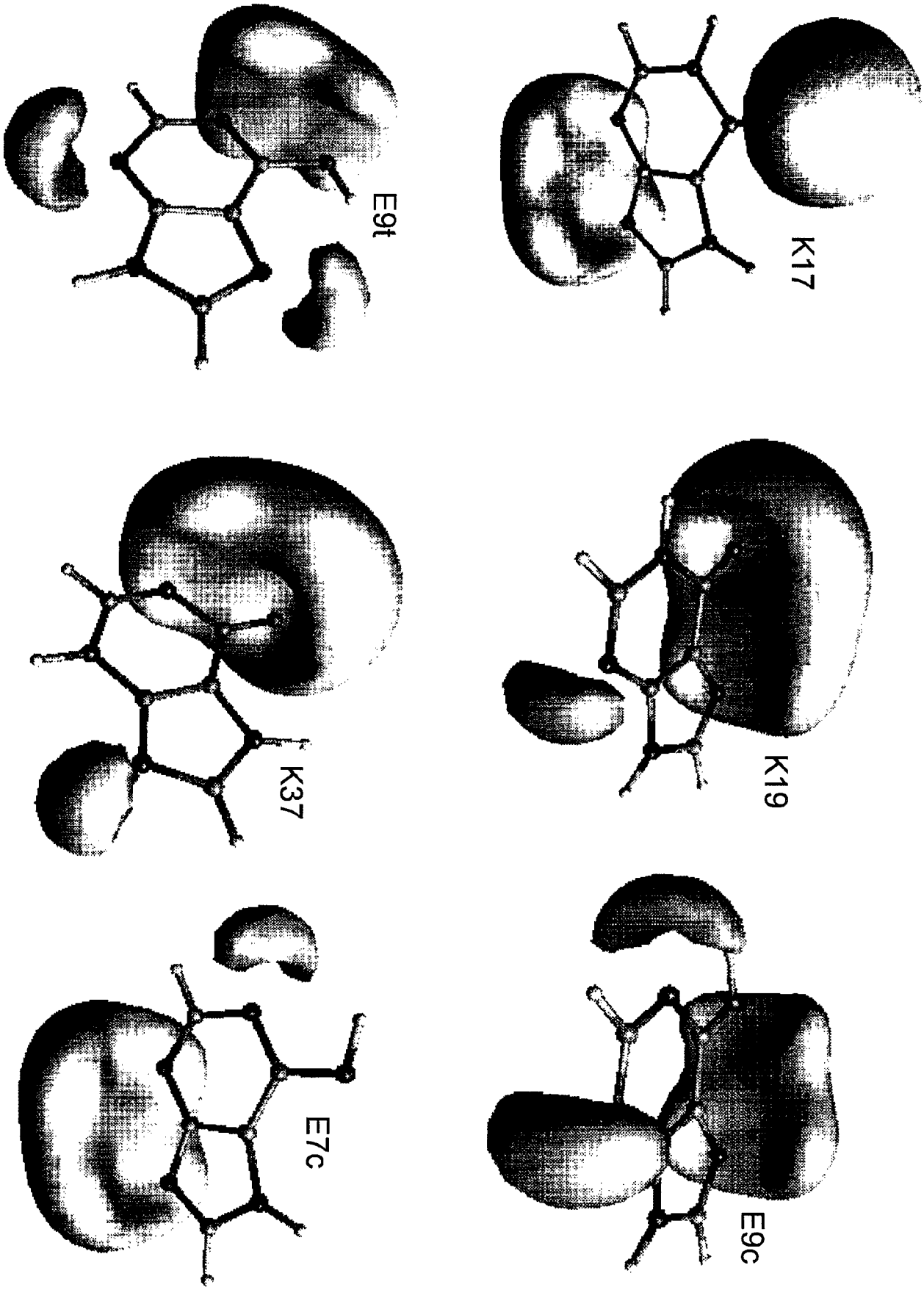
Vibrational modes analysis for the N(3)-H/N(7)-H ketonic tautomer and the cis-N(7) enolic tautomer.

| N(3)-H/N(7)-H ketonic tautomer | | | cis-N(7)-H enolic tautomer | | |
|---|---|---|---|---|---|
| $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments | $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments |
| 1244.80 | 16.21 | Rings vib.<br>C(8) – H/N(3) – H vib. | 1259.98 | 51.12 | Rings vib.<br>$\delta$ COH* |
| 1160.29 | 23.37 | Rings vib.<br>C(8) – H/N(7) – H vib. | 1211.02 | 32.13 | Rings vib.<br>C(8) – H/N(7) – H vib.<br>$\delta$ COH* |
| 1081.10 | 27.79 | Rings vib.<br>N(7) – H/N(3) – H vib. | 1108.34 | 15.42 | Rings vib.<br>$\delta$ COH* |
| 1049.79 | 18.26 | Rings vib.<br>N(7) – H vib. | 1063.41 | 69.39 | Rings vib.<br>N(7) – H vib.<br>$\delta$ COH* |
| 998.61 | 43.67 | Rings vib.<br>N(7) – H vib. | 1029.02 | 117.08 | Rings vib.<br>N(7) – H/C(8) – H vib.<br>$\delta$ COH* |
| 921.14 | 5.33 | Rings vib. | 914.07 | 9.55 | C(2)-H vib.[a] |
| 881.73 | 11.89 | C(2)-H vib.[a] | 907.56 | 2.66 | Rings vib. |
| 863.36 | 1.51 | Rings vib. | 849.18 | 18.09 | Rings vib.<br>$\nu$ C – O |
| 775.49 | 26.41 | C(8)-H vib. [a] | 812.08 | 23.62 | C(8)-H vib.[a] |
| 749.26 | 0.39 | C(8) – H vib.[a]<br>Rings vib. | 767.20 | 4.11 | C(8) – H vib.[a]<br>Rings vib. |
| 688.44 | 3.45 | Rings vib. | 700.15 | 1.58 | Rings vib.<br>$\nu$ C – O |
| 674.33 | 2.83 | Rings vib. [a] | 663.68 | 7.77 | Rings vib.[a] |
| 628.42 | 7.72 | N(7) – H vib.[a]<br>Rings vib. | 613.38 | 5.25 | Rings vib.[a]<br>N(7) – H vib.<br>$\delta$ OH |
| 601.59 | 1.14 | Rings vib. | 589.37 | 0.73 | Rings vib. |
| 553.09 | 26.37 | N(3)-H vib. [a] | 559.04 | 0.12 | C(2) – H vib.[a]<br>Rings vib. |
| 521.42 | 121.52 | N(7)-H vib. [a] | 521.33 | 0.30 | Rings vib. |

Vibrational modes analysis for the N(3)-H/N(7)-H ketonic tautomer and the cis-N(7) enolic tautomer (Continuation).

| N(3)-H/N(7)-H ketonic tautomer | | | cis-N(7)-H enolic tautomer | | |
|---|---|---|---|---|---|
| $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments | $\bar{\nu}$ ($cm^{-1}$) | $I$ (KM/mol) | Assignments |
| 506.37 | 3.51 | Pirimidinic ring vib. | 521.10 | 118.68 | $\delta$ OH/$\nu$OH[a] Imidazolic ring vib. |
| 485.18 | 3.89 | Pirimidinic ring vib. | 503.82 | 0.55 | Pirimidinic ring vib. |
| 429.79 | 38.94 | N(3) – H vib.[a] Rings vib. | 425.56 | 88.26 | N(7) – H vib.[a] Imidazolic ring vib. $\delta$ OH |
| 287.24 | 21.91 | Rings vib. [a] | 288.08 | 4.49 | Rings vib. |
| 285.49 | 14.88 | Pirimidinic ring vib. $\nu$ C = O | 279.07 | 12.57 | Rings vib. $\delta$ C – O |
| 166.74 | 0.21 | Rings vib. [a] | 202.52 | 7.89 | Rings vib.[a] $\delta$ OH |
| 124.48 | 3.86 | $\delta$ C = O[a] Rings vib. | 156.56 | 3.01 | Rings vib.[a] N(7) – H vib. $\delta$ COH |

Vibrational modes analysis for the N(3)-H/N(7)-H ketonic tautomer and the cis-N(7) enolic tautomer (Continuation).


E9t
K17
K37
K19
E7c
E9c