Spectroscopic (FT-IR & FT-Raman), Fukui function and molecular docking analysis of 6-amino-7,9-dihydropurine-8-thione by DFT approach

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Supplementary material

Table S1. Geometrical optimized parameters of ADHPT

Atoms	DFT	Atoms	DFT
Bond length		**Bond angle**	
S1-C10	1.659	S1-C10-N2	127.5
N2-C7	1.393	S1-C10-N3	127.8
N2-C10	1.38	C7-N2-C10	110.8
N2-H12	1.007	N2-C7-C6	106.6
N3-C8	1.379	N2-C7-C9	136.4
N3-C10	1.383	N2-C10-N3	104.6
N3-H13	1.009	C8-N3-C10	111.4
N4-C8	1.326	N3-C8-N4	127.8
N4-C11	1.339	N3-C8-C7	106.5
N5-C9	1.345	C8-N4-C11	112.4
N5-C11	1.333	N4-C8-C7	125.6
N6-C9	1.372	N4-C11-N5	127.7
N6-H15	1.008	C9-N5-C11	119
N6-H16	1.01	N5-C9-N6	117.7
C7-C8	1.396	N5-C9-C7	118.2
C7-C9	1.396	N5-C11-H14	116
C11-H14	1.085	N6-C9-C7	124

Table S2. Observed and calculated vibrational assignments of ADHPT

Mode No.	Wavenumber (cm^{-1})				Intensity				Assignments (PED≥10%)[d]
	Experimental		Theoretical		FT-IR		Raman		
	FT-IR	Raman	Unscaled	Scaled[a]	Relative[b]	Absolute	Relative[b]	Absolute	
42	–	–	3750	3604	6.5	6	45	25	νNH(98)
41	3482	–	3665	3522	7.7	8	98	54	νNH(99)
40	–	–	3651	3509	13.6	14	91	49	νNH(99)
39	3345	3280	3618	3477	14.8	15	184	100	νNH(98)
38	2854	2976	3177	3053	1.8	2	163	89	νCH(100)
37	–	1662	1674	1609	74.4	74	18	10	νCC(48)+βHNH(10)+βCCN(10)
36	1636	1586	1634	1570	17.6	18	53	29	νNC(64)
35	1541	1537	1624	1561	1.0	1	4	2	βHNH(67)
34	1482	1479	1502	1444	100.0	100	41	22	νNC(15)+βHNC(34)+βHNC(20)
33	1436	1440	1490	1431	8.4	8	5	3	νNC(48)+βHCN(25)
32	–	1380	1468	1411	15.2	15	146	79	νNC(58)+βCNC(12)+βHCN(11)
31	1339	1372	1387	1333	10.7	11	3	2	νNC(12)+βHCN(47)
30	–	–	1365	1312	0.3	0	19	11	νNC(32)+HCN(31)
29	–	–	1336	1284	7.2	7	29	16	νNC(77)
28	1262	1260	1313	1261	9.4	9	3	2	νNC(56)
27	1230	1204	1261	1212	1.0	1	47	26	νNC(46)+βHCN(13)
26	–	1136	1232	1184	0.3	0	46	25	νSC(12)+HCN(11)
25	1166	–	1156	1111	12.9	13	8	4	βHNC(18)+βHNC(14)+NC(31)
24	1072	1034	1129	1085	14.5	14	7	4	βHNC(16)+ βHNC(21)
23	595	973	996	957	2.0	2	12	6	βHNC(50)+ νCC(10)
22	837	–	982	943	3.2	3	25	14	νNC(35)+CNC(18)
21	–	922	972	934	0.5	1	0	0	τH-C-N-C(89)
20	–	–	902	867	2.3	2	7	4	βCNC(62)
19	790	758	780	750	1.0	1	11	6	νSC(56)
18	776	738	775	745	1.8	2	1	0	τH-N-C-C(84)
17	669	–	677	651	0.8	1	0	0	τH-N-C-N(86)
16	–	648	648	623	0.3	0	2	1	τ HNCN(89)
15	598	–	635	610	1.5	2	4	2	βCCN(72)
14	–	–	571	548	0.9	1	17	9	βCCN(42)
13	558	–	561	539	0.8	1	1	0	τ N-C-C-N(82)
12	–	525	549	527	13.7	14	0	0	τ H-N-C-N(93)
11	–	–	543	521	0.4	0	3	1	βCCN(62)
10	–	478	474	455	0.1	0	0	0	τ H-N-C-N(80)

9	420	−	435	418	0.4	0	16	9	νNC(13)+ βCCN(16)
8	−	368	400	385	9.8	10	1	0	τ H-N-C-S(70)
7	−	−	340	327	0.8	1	5	3	βCCN(73)
6	−	−	283	272	0.4	0	1	0	τ H-N-C-N(83)
5	−	232	255	245	1.1	1	2	1	τ H-N-C-N(64)
4	−	−	193	186	0.5	1	6	3	τ N-C-C-N(11)
3	−	134	145	139	0.1	0	0	0	βNCS(74)
2	−	−	97	93	0.0	0	0	0	τ C-N-C-C(72)
1	−	−	-312	-300	22.2	22	0	0	τ C-N-C-S(80)

ν-Stretching, β- deformation, τ -Torsion.

a Scaling factor 0.961 for B3LYP/6-311++G (d,p)

b Relative absorption intensities normalized with highest peak absorption equal to 100.

c Relative Raman intensities normalized to 100 (R; Real, A; Absolute).