

Overruling the energy gap law: Fast triplet formation in 6-azauracil

Electronic Supplementary Information

Mihajlo Etinski and Christel Marian

Heinrich-Heine-University Düsseldorf,
Institute of Theoretical and Computational Chemistry
Universitätsstraße 1, 40225 Düsseldorf, Germany.
Fax: +49 211 8113466; Tel: +49 211 8113209
E-mail: Christel.Marian@uni-duesseldorf.de

April 1, 2010

Table 1: Vibrational spectrum of the ground state state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies). Wavenumbers ν are given in cm^{-1} , intensities I in km/mol .

ν	I
126	0.97
145	1.19
368	20.81
392	6.66
506	4.92
521	21.15
543	8.62
607	44.99
704	133.41
725	18.89
732	8.89
744	1.50
886	19.27
971	26.96
1003	7.12
1127	25.28
1237	29.31
1338	33.74
1365	10.22
1406	87.14
1439	54.04
1581	14.24
1733	286.99
1798	518.09
3263	0.09
3584	67.76
3631	118.88

Table 2: Vibrational spectrum of the S_1 state state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies). Wavenumbers ν are given in cm^{-1} , intensities I in km/mol .

ν	I
103	0.63
183	0.06
302	5.86
314	5.06
409	69.32
472	13.38
494	3.15
546	9.07
589	12.46
656	79.88
681	23.19
695	1.25
768	45.28
915	17.94
968	20.72
1021	32.62
1107	3.98
1169	5.44
1260	0.92
1297	3.91
1429	8.24
1435	1.14
1602	211.85
1770	388.46
3279	5.00
3601	75.72
3619	157.15

Table 3: Vibrational spectrum of the S_2 state state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies). Wavenumbers ν are given in cm^{-1} , intensities I in km/mol .

ν	I
43	0.56
194	1.19
310	11.88
355	10.44
371	24.51
488	22.71
501	21.60
511	2.31
563	0.10
627	55.30
670	50.46
696	121.51
703	60.51
813	11.11
895	8.09
928	487.40
1084	31.89
1100	0.60
1225	61.10
1269	46.71
1371	149.71
1408	24.64
1616	68.50
1737	232.91
3236	1.28
3583	205.26
3595	99.77

Table 4: Vibrational spectrum of the T_1 state state obtained at RI-CC2/cc-pVDZ level (unscaled frequencies). Wavenumbers ν are given in cm^{-1} , intensities I in km/mol .

ν	I
127	1.83
155	1.25
224	2.32
364	18.19
436	8.95
481	12.02
513	15.41
520	10.48
573	10.73
660	132.04
692	10.34
712	84.28
729	10.92
950	28.09
977	9.36
1013	12.06
1206	40.27
1245	3.64
1323	145.94
1358	1.12
1396	110.36
1424	60.12
1637	113.46
1769	280.24
3260	1.67
3557	69.07
3596	78.38

Table 5: Cartesian coordinates/bohr of the ground state minimum obtained at RI-CC2/cc-pVDZ level

-1.74610099736496	-2.22240265834325	0.00449565927163	c
1.04380765341883	-2.32412964268841	-0.00234588751951	c
2.11572577304878	0.10751366537799	-0.00119438050326	n
0.82956298515604	2.41214101722268	0.00553295218914	c
-1.79204276381764	2.06387091765626	0.01355038214799	n
-3.09282819734742	-0.14023042659925	0.01202440802523	n
1.83958958452372	4.49581537459581	0.00484352223484	o
2.32658155756143	-4.26488628454951	-0.00851159800297	o
-2.79455216344083	-4.00208925911174	0.00333103347986	h
-2.86851142686696	3.65789742855908	0.01819485140458	h
4.04389471091239	0.21864498496745	-0.00677148077657	h

Table 6: Cartesian coordinates/bohr of the S_1 state obtained at RI-CC2/cc-pVDZ level

-1.70942743306936	-2.28862676386382	0.01171803574604	c
0.85186934253273	-2.18433362413726	0.00304030842125	c
2.11879899612192	0.08546595015361	0.00540273369754	n
0.81137827666896	2.40924641302505	0.01350208669795	c
-1.77960155935168	2.06066459904651	0.02315894080454	n
-3.21179872531814	-0.09522472029197	0.02304793827355	n
1.89301875972419	4.46794230004381	0.01235157021997	o
2.63879617184379	-4.20210264894317	-0.00908114690792	o
-2.73969468817620	-4.07409795610917	0.01066363238671	h
-2.80045655928674	3.69613248188546	0.02979266612826	h
4.04302727571830	0.15860473290155	-0.00452307249332	h

Table 7: Cartesian coordinates/bohr of the S_2 state obtained at RI-CC2/cc-pVDZ level

-1.71827507408612	-2.24397766518739	0.01233487758568	c
0.94769711480994	-2.43280073654303	0.00179277976845	c
2.13383170529868	0.19901431998794	0.00433266655245	n
0.74490682054897	2.27973110212464	0.01359962671832	c
-1.76229403339219	2.12172237235798	0.02286910927231	n
-3.31854266039105	-0.16204656007902	0.02398871968691	n
1.74363854174153	4.60190904005255	0.01450380274673	o
2.44222912958946	-4.24743837997651	-0.00897205844489	o
-2.76104184321613	-4.03251594913419	0.01150692493834	h
-2.73262450517248	3.79305171030558	0.02980335552034	h
4.05821674617707	0.35482825420333	-0.00325525027252	h

Table 8: Cartesian coordinates/bohr of the T_1 state obtained at RI-CC2/cc-pVDZ level

-1.70543259811873	-2.22687115289721	0.05256993108285	c
1.03026286184038	-2.31744010721149	0.09054337463554	c
2.09747813119421	0.12995182046546	0.37693092483039	n
0.77876402984206	2.34280092007962	-0.13161907485166	c
-1.89425265511141	2.01206264772269	-0.09336157908310	n
-3.12399577475616	-0.03071173985523	0.88344339396988	n
1.72120608700431	4.42655751619203	-0.49253711953501	o
2.36524653906037	-4.21703605018496	-0.19608731641017	o
-2.77917281453484	-3.78287057822387	-0.77974663553158	h
-2.84376858923679	3.68819780655726	0.07914263401925	h
4.01715552887198	0.25434139281412	0.23008822353881	h