

Thermochemical Studies of Pyrazolide

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Supporting Information

Harmonic vibrational frequencies of $\tilde{X}^1A_1$ 1-pyrazolide, $\tilde{X}^2A_2$, $\tilde{A}^2B_1$, and $\tilde{B}^2B_2$ 1-pyrazolyl obtained at the B3LYP/6-311++G(d,p) level.

Harmonic vibrational frequencies of $\tilde{X}^1A'$ 5-pyrazolide and $\tilde{X}^2A'$ 5-pyrazolyl obtained at the B3LYP/6-311++G(d,p) level.

Harmonic vibrational frequencies (cm⁻¹) at the B3LYP/6-311++G(d,p) level of theory.

mode	symmetry	1-pyrazolide	1-pyrazolyl		
		$\tilde{X}^1A_1$	$\tilde{X}^2A_2$	$\tilde{A}^2B_1$	$\tilde{B}^2B_2$
1	a_1	3194	3269	3234	3285
2		3148	3235	3212	3243
3		1471	1510	1521	1609
4		1215	1390	1300	1391
5		1127	1121	1054	1199
6		1026	1007	924	1075
7		930	912	786	913
8	a_2	756	835	859	794
9		693	564	188	286i
10	b_1	784	860	882	863
11		696	700	705	765
12		631	408	480	101
13	b_2	3151	3239	3216	3279
14		1405	1336	1477	1422
15		1363	1287	1283	1283
16		1165	990	1179	1161
17		1031	950	946	1039
18		914	599	539	627

Harmonic vibrational frequencies (cm⁻¹) at the B3LYP/6-311++G(d,p) level of theory.

mode	symmetry	$\tilde{X}^1A'$ 5-pyrazolide	$\tilde{X}^2A'$ 5-pyrazolyl
1	a'	3654	3676
2		3175	3275
3		3149	3232
4		1492	1526
5		1391	1442
6		1348	1372
7		1247	1317
8		1178	1261
9		1104	1162
10		1056	1048
11		1030	1038
12		922	915
13		901	886
14	a''	840	884
15		753	770
16		696	670
17		650	572
18		527	440