

Comparison of structural fits for pyrazole:

	Parent	N1-D	3-D	4-D	5-D	15N1	15N2	13C3	13C4	13C5
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JPCA2015:										
A0	9618.770	9455.230	9435.783	9566.176	9537.304	9488.641	9618.304	9457.566	9582.358	9571.674
B0	9412.535	8859.733	8774.190	8617.847	8677.868	9339.851	9180.010	9340.099	9193.394	9223.004
C0	4755.853	4572.847	4545.189	4532.324	4542.381	4705.424	4695.610	4697.835	4690.511	4695.634
Ae-A0	78.418	81.054	77.298	81.474	75.831	81.197	77.791	75.230	80.055	75.824
Be-B0	79.703	65.764	70.934	66.561	71.890	75.122	77.420	79.869	75.078	79.168
Ce-C0	41.431	37.997	38.714	38.448	38.618	40.925	40.683	40.662	40.617	40.657
Ae*	9697.604	9536.935	9513.701	9648.161	9613.613	9570.392	9696.509	9533.327	9662.884	9647.927
Be	9492.919	8925.885	8845.526	8684.907	8750.287	9415.506	9258.078	9420.518	9269.072	9302.812
Ce	4797.119	4610.691	4583.751	4570.622	4580.849	4746.187	4736.131	4738.335	4730.967	4736.130
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dA (o-c)	-0.154	0.012	0.098	0.035	-0.012	0.153	-0.059	0.239	0.117	-0.008
dB (o-c)	0.021	-0.053	-0.056	-0.018	-0.025	-0.189	-0.216	-0.212	-0.018	0.125
dC (o-c)	0.002	0.030	0.031	0.011	0.011	0.018	-0.051	0.048	0.049	-0.083
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STRFIT:										
dA (o-c)	-0.1820	-0.0072	0.0748	0.0270	-0.0168	0.1990	-0.0847	0.2256	0.0699	-0.0688
dB (o-c)	-0.0020	-0.0761	-0.0774	-0.0247	-0.0324	-0.2265	-0.1598	-0.2573	-0.0518	0.0056
dC (o-c)	-0.0111	0.0200	0.0203	0.0070	0.0081	0.0198	-0.0424	0.0334	0.0291	0.0015

\* Ae = A0 + (Ae-A0) - A\_el., where A\_el = 0.000544617 g\_aa Ae etc.

Fits to all A,B,C:	STRFIT, only (Be-B0) corrections*	STRFIT** the same input data with (Be-B0) and g_bb corrections	JPCA2015**
R( 6, 1) =	1.0008 +- 0.0013	1.001246 +- 0.000348	N1-H 1.0014(4)
R( 2, 1) =	1.3447 +- 0.0019	1.343679 +- 0.000517	N1-N2 1.3431(6)
R( 3, 2) =	1.3287 +- 0.0020	1.328724 +- 0.000565	N2=C3 1.3286(7)
R( 5, 1) =	1.3515 +- 0.0017	1.352075 +- 0.000480	N1-C5 1.3523(6)
R( 4, 3) =	1.4091 +- 0.0018	1.409276 +- 0.000507	C3-C4 1.4093(6)
R( 7, 3) =	1.0768 +- 0.0012	1.075579 +- 0.000326	C3-H 1.0755(8)
R( 8, 4) =	1.0744 +- 0.0011	1.073673 +- 0.000311	C4-H 1.0736(4)
R( 9, 5) =	1.0762 +- 0.0015	1.074432 +- 0.000406	C5-H 1.0740(5)
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A( 3, 2, 1) =	104.09 +- 0.10	104.1604 +- 0.0289	N1-N2-C3 104.18(3)
A( 4, 3, 2) =	111.94 +- 0.13	111.8999 +- 0.0358	N1-C3-C4 111.90(5)
A( 5, 1, 2) =	113.22 +- 0.15	113.2151 +- 0.0401	N2-N1-C5 113.24(5)
A( 6, 1, 2) =	118.62 +- 0.39	118.9502 +- 0.1084	H-N1-N2 118.97(11)
A( 7, 3, 2) =	119.42 +- 0.47	119.4708 +- 0.1354	N2-C3-H 119.49(14)
A( 8, 4, 3) =	128.23 +- 0.46	128.2860 +- 0.1298	C3-C4-H 128.32(13)
A( 9, 5, 1) =	121.50 +- 0.39	121.7950 +- 0.1084	N1-C5-H 121.84(11)
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Chi-squared	0.0001636138	0.0000124847	
Deviation of fit	0.003303	0.000912	

\* - (Be-B0) corrections calculated at the MP2/cc-pVTZ level

\*\* - (Be-B0) and B\_el corrections calculated at the B3LYP/6-31+G(3df,2pd) level