

# Electronic Supporting Information

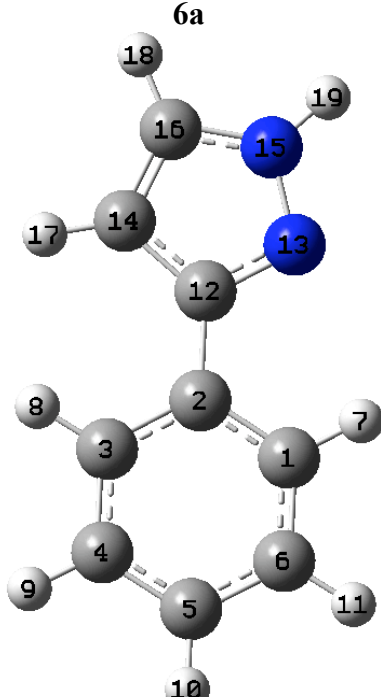
## A Theoretical and Experimental NMR Study of the Tautomerism of two Phenylene-bis-C-Substituted Pyrazoles

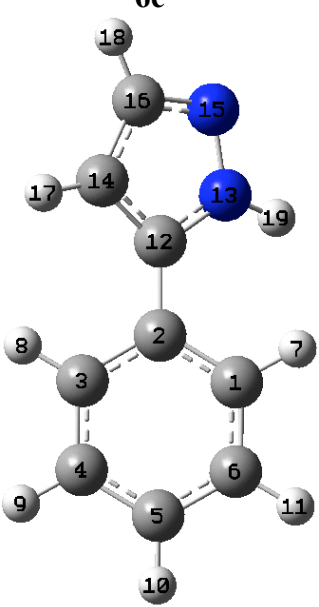
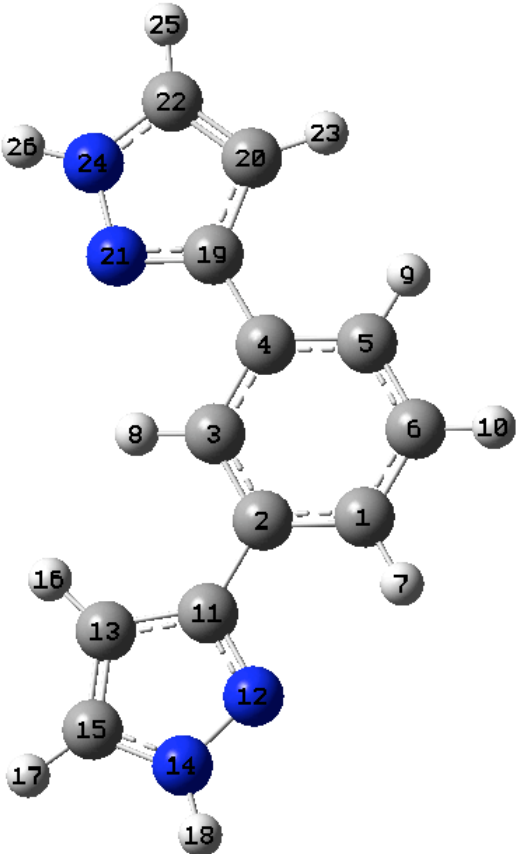
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Energies of the optimized structure at the B3LYP/6-311++G(d,p) computational level.

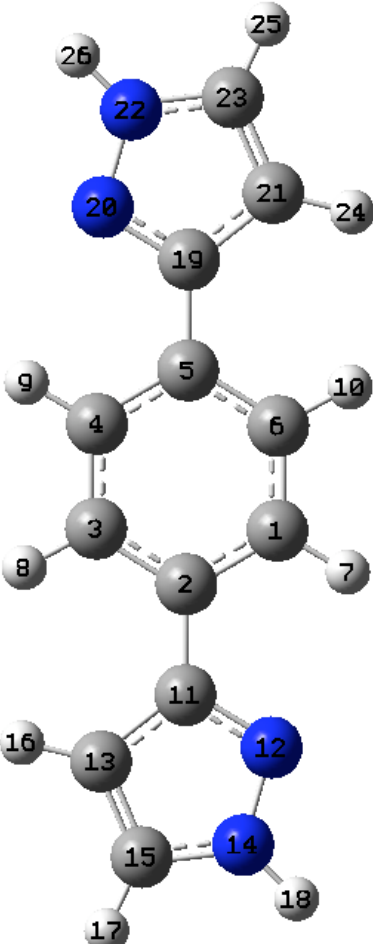
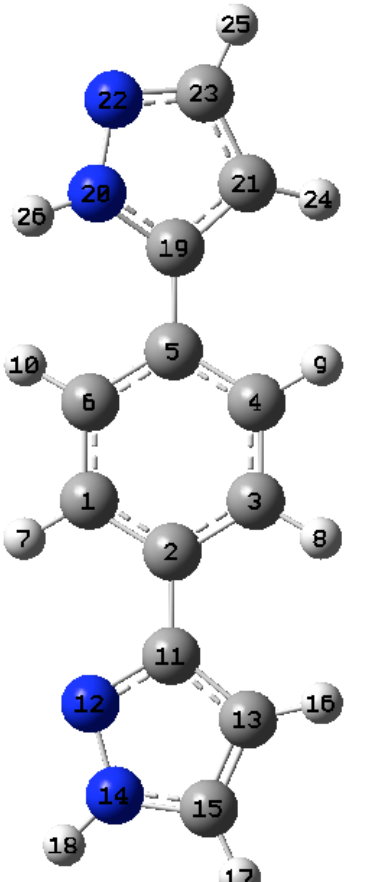
Molecule	Gas Phase		DMSO	
	Etotal (hartree)	Erel(kJ/mol)	E total + $\Delta G$ Solvation	Erel(kJ/mol)
<b>1a</b>	-682.450982327	0.00	-682.473389	0.00
<b>1b</b>	-682.450555081	1.12	-682.471605	4.68
<b>1c</b>	-682.448972332	5.28	-682.469908	9.14
<b>2a</b>	-682.451328869	0.00	-682.474428	0.00
<b>2b</b>	-682.451102268	0.59	-682.473021	3.69
<b>2c</b>	-682.449598336	4.54	-682.471127	8.67
<b>6a</b>	-457.381091035	0.00	-457.393745	0.00
<b>6c</b>	-457.380550295	1.42	-457.392315	3.75

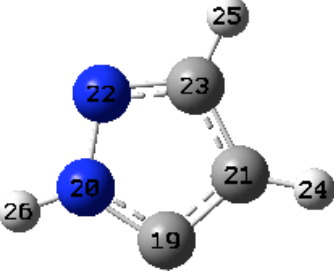
### Absolute chemical shieldings

Structure	Gas Phase	DMSO
 <p><b>6a</b></p>	1 C 52.4833	1 C 54.2521
	2 C 43.1683	2 C 43.1459
	3 C 53.6403	3 C 53.0627
	4 C 49.9652	4 C 48.7063
	5 C 50.7791	5 C 50.2666
	6 C 49.2492	6 C 48.9010
	7 H 23.2499	7 H 23.2031
	8 H 24.0781	8 H 23.6843
	9 H 24.4667	9 H 24.0883
	10 H 24.5974	10 H 24.2561
	11 H 24.4341	11 H 24.1160
	12 C 24.3252	12 C 25.1924
	13 N -71.5407	13 N -58.9395
	14 C 77.3494	14 C 77.2859
	15 N 42.5667	15 N 34.7673
	16 C 51.4057	16 C 47.1549
	17 H 25.0971	17 H 24.7220
	18 H 24.4795	18 H 23.9047
	19 H 22.7862	19 H 21.6180

<p style="text-align: center;"><b>6c</b></p> 	<p>1 C 54.6065                  2 C 45.3612                  3 C 50.7961                  4 C 48.4157                  5 C 50.2293                  6 C 48.7773                  7 H 24.3963                  8 H 24.1459                  9 H 24.3393                  10 H 24.4702                  11 H 24.3608                  12 C 33.8519                  13 N 41.6453                  14 C 75.6376                  15 N -81.3965                  16 C 36.2958                  17 H 25.3828                  18 H 24.2515                  19 H 22.5867</p>	<p>1 C 52.7625                  2 C 46.4345                  3 C 50.5318                  4 C 48.2247                  5 C 48.8128                  6 C 48.1673                  7 H 23.9223                  8 H 23.8455                  9 H 23.9941                  10 H 24.0829                  11 H 23.9881                  12 C 31.8875                  13 N 37.5711                  14 C 75.3188                  15 N -63.2176                  16 C 35.9664                  17 H 24.9798                  18 H 24.0108                  19 H 21.5660</p>
<p style="text-align: center;"><b>1a</b></p> 	<p>1 C 53.1946                  2 C 43.2431                  3 C 56.1319                  4 C 44.2386                  5 C 54.5238                  6 C 49.7286                  7 H 23.4025                  8 H 22.8991                  9 H 24.2763                  10 H 24.4752                  11 C 23.9005                  12 N -71.0516                  13 C 76.0761                  14 N 43.1309                  15 C 51.3732                  16 H 24.8401                  17 H 24.4663                  18 H 22.7838                  19 C 24.0439                  20 C 76.8849                  21 N -70.1966                  22 C 51.5830                  23 H 25.1079                  24 N 43.3716                  25 H 24.4836                  26 H 22.7704</p>	<p>1 C 54.9908                  2 C 43.1956                  3 C 58.0276                  4 C 43.3252                  5 C 53.9102                  6 C 48.4504                  7 H 23.3518                  8 H 22.8826                  9 H 23.8742                  10 H 24.0996                  11 C 25.0644                  12 N -59.3066                  13 C 76.5192                  14 N 34.6943                  15 C 46.8739                  16 H 24.5498                  17 H 23.8772                  18 H 21.5766                  19 C 25.2917                  20 C 76.6755                  21 N -59.2161                  22 C 47.1616                  23 H 24.7327                  24 N 34.8090                  25 H 23.8925                  26 H 21.5479</p>

<p style="text-align: center;"><b>1b</b></p>	<p>1 C 52.8343                  2 C 41.9431                  3 C 54.5089                  4 C 45.9626                  5 C 55.7573                  6 C 48.3463                  7 H 23.3264                  8 H 23.8800                  9 H 24.5453                  10 H 24.3512                  11 C 24.7572                  12 N -72.8026                  13 C 77.0140                  14 N 41.6381                  15 C 51.0441                  16 H 25.0452                  17 H 24.4246                  18 H 22.6880                  19 C 33.3056                  20 C 75.9683                  21 N 41.1349                  22 C 36.5786                  23 H 25.3665                  24 N -80.6126                  25 H 24.2470                  26 H 22.5672</p>	<p>1 C 53.6993                  2 C 42.1913                  3 C 54.4263                  4 C 46.1831                  5 C 53.7304                  6 C 47.6171                  7 H 23.2233                  8 H 23.6471                  9 H 24.0590                  10 H 23.9790                  11 C 25.5617                  12 N -60.4414                  13 C 77.0699                  14 N 33.9282                  15 C 47.0009                  16 H 24.6933                  17 H 23.8648                  18 H 21.5185                  19 C 31.8435                  20 C 75.1644                  21 N 37.0194                  22 C 36.0484                  23 H 24.9319                  24 N -63.5074                  25 H 23.9851                  26 H 21.5480</p>
<p style="text-align: center;"><b>1c</b></p>	<p>1 C 51.6432                  2 C 44.3953                  3 C 58.7647                  4 C 44.3954                  5 C 51.6436                  6 C 47.4468                  7 H 24.2403                  8 H 24.4676                  9 H 24.2403                  10 H 24.2850                  11 C 34.2928                  12 N 41.6345                  13 C 74.9749                  14 N -83.1742                  15 C 36.2062                  16 H 25.3461                  17 H 24.2109                  18 H 22.5832                  19 C 34.2931                  20 C 74.9737                  21 N 41.6347                  22 C 36.2055                  23 H 25.3461                  24 N -83.1750                  25 H 24.2108                  26 H 22.5832</p>	<p>1 C 50.3376                  2 C 45.3554                  3 C 55.8063                  4 C 45.3559                  5 C 50.3382                  6 C 47.3146                  7 H 23.8740                  8 H 23.8754                  9 H 23.8735                  10 H 23.9088                  11 C 32.3331                  12 N 37.2237                  13 C 74.5895                  14 N -64.7282                  15 C 36.0066                  16 H 24.9358                  17 H 23.9802                  18 H 21.5532                  19 C 32.3364                  20 C 74.5877                  21 N 37.2330                  22 C 36.0060                  23 H 24.9359                  24 N -64.7402                  25 H 23.9802                  26 H 21.5570</p>

<p style="text-align: center;"><b>2a</b></p> 	<p>1 C 52.8430                  2 C 44.4677                  3 C 53.2393                  4 C 52.8430                  5 C 44.4677                  6 C 53.2393                  7 H 23.2914                  8 H 24.1253                  9 H 23.2914                  10 H 24.1253                  11 C 24.1013                  12 N -70.9540                  13 C 76.8180                  14 N 42.8735                  15 C 51.4426                  16 H 25.0922                  17 H 24.5104                  18 H 22.7777                  19 C 24.1013                  20 N -70.9540                  21 C 76.8180                  22 N 42.8735                  23 C 51.4426                  24 H 25.0922                  25 H 24.5104                  26 H 22.7777</p>	<p>1 C 53.7600                  2 C 44.3317                  3 C 52.7795                  4 C 53.7599                  5 C 44.3316                  6 C 52.7795                  7 H 23.1972                  8 H 23.7503                  9 H 23.1972                  10 H 23.7503                  11 C 25.1938                  12 N -58.8741                  13 C 76.7425                  14 N 34.6536                  15 C 47.0331                  16 H 24.7282                  17 H 23.9271                  18 H 21.5867                  19 C 25.1923                  20 N -58.8752                  21 C 76.7425                  22 N 34.6550                  23 C 47.0360                  24 H 24.7284                  25 H 23.9270                  26 H 21.5868</p>
<p style="text-align: center;"><b>2b</b></p> 	<p>1 C 51.8158                  2 C 43.9577                  3 C 52.7152                  4 C 51.5350                  5 C 47.1917                  6 C 54.5469                  7 H 23.2526                  8 H 24.0194                  9 H 24.1645                  10 H 24.3919                  11 C 25.1979                  12 N -72.0200                  13 C 76.9623                  14 N 41.8399                  15 C 50.9721                  16 H 25.0770                  17 H 24.4610                  18 H 22.7354                  19 C 33.8755                  20 N 42.0526                  21 C 76.1416                  22 N -80.6162                  23 C 36.4356                  24 H 25.3784                  25 H 24.2574                  26 H 22.5445</p>	<p>1 C 53.3266                  2 C 43.2709                  3 C 52.3648                  4 C 50.4158                  5 C 48.0286                  6 C 52.7476                  7 H 23.1623                  8 H 23.6139                  9 H 23.8074                  10 H 23.9246                  11 C 25.9832                  12 N -60.2455                  13 C 76.7150                  14 N 33.9509                  15 C 46.9180                  16 H 24.6866                  17 H 23.8965                  18 H 21.5583                  19 C 32.2734                  20 N 38.1054                  21 C 75.6012                  22 N -63.0022                  23 C 35.9360                  24 H 24.9589                  25 H 24.0020                  26 H 21.5434</p>

2c	1 C 53.9303	1 C 52.2487
	2 C 47.1339	2 C 46.9520
	3 C 50.5022	3 C 49.9546
	4 C 53.9306	4 C 52.2505
	5 C 47.1325	5 C 46.9511
	6 C 50.5027	6 C 49.9552
	7 H 24.3277	7 H 23.8547
	8 H 24.1223	8 H 23.7426
	9 H 24.3280	9 H 23.8552
	10 H 24.1223	10 H 23.7425
	11 C 34.7735	11 C 32.8249
	12 N 41.9898	12 N 37.8041
	13 C 75.3957	13 C 74.7952
	14 N -82.8067	14 N -64.5032
	15 C 36.2018	15 C 35.8372
	16 H 25.4205	16 H 24.9169
	17 H 24.2605	17 H 23.9873
	18 H 22.4740	18 H 21.5324
	19 C 34.7736	19 C 32.8264
	20 N 41.9881	20 N 37.8054
	21 C 75.3933	21 C 74.7933
	22 N -82.8075	22 N -64.5026
	23 C 36.2007	23 C 35.8358
	24 H 25.4206	24 H 24.9169
	25 H 24.2606	25 H 23.9872
	26 H 22.4740	26 H 21.5326