Supporting Information

Pure rotational spectrum and model calculations of anisole-ammonia

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Completion of the Reference:

[27] GAUSSIAN03, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, **2003**.

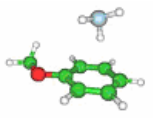
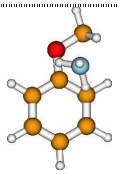
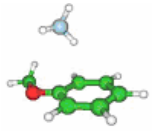
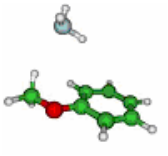
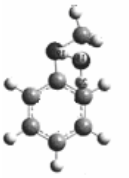
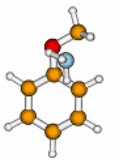
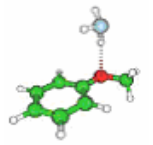
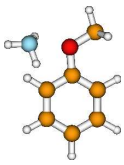
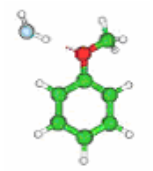
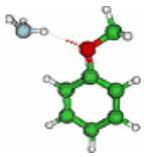
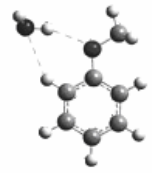
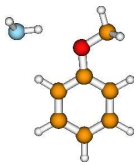
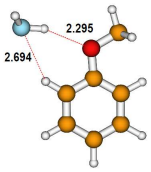
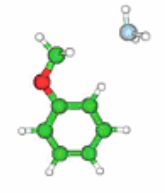
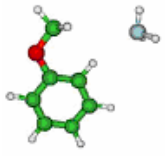
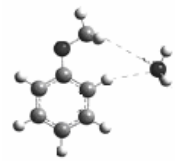
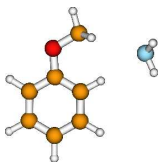
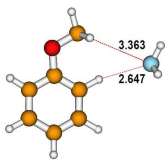
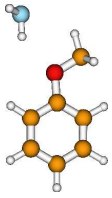
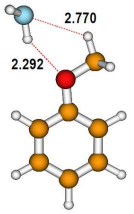
Table S1. Measured transition frequencies (ν, MHz) and, in parethesis, observed – calculated values ($\Delta\nu$, kHz, rounded to the unit) for the two observed conformers of Glycidol dimer Table: Experimental rotational frequencies of anisole···NH_3.

J"(K_{-1}",K_1") - J'(K_{-1}',K_1')	F"-F'	ν / MHz
2 (2, 1) - 1 (1, 0)	3 - 2	7399.467
	2 - 1	7399.797
	1 - 0	7398.988
	1 - 1	7399.762
3 (2, 2) - 2 (1, 1)	4 - 3	9400.929
	3 - 2	9401.279
	2 - 1	9400.733
3 (2, 1) - 2 (1, 2)	4 - 3	9702.429
	3 - 2	9702.022
	2 - 1	9702.640
3 (3, 1) - 2 (2, 0)	4 - 3	11708.358
	3 - 2	11708.391
	2 - 1	11708.347
3 (1, 2) - 2 (0, 2)	4 - 3	7639.311
	3 - 2	7638.941
	2 - 1	7639.445
4 (0, 4) - 3 (1, 3)	5 - 4	7475.790
	4 - 3	7475.558
	3 - 2	7475.882
4 (1, 4) - 3 (0, 3)	5 - 4	9015.898
	4 - 3	9016.212
	3 - 2	9015.822
4 (2, 3) - 3 (1, 2)	5 - 4	11356.080
	4 - 3	11356.434
	3 - 2	11355.949
4 (2, 2) - 3 (1, 3)	5 - 4	11986.069
	4 - 3	11985.589
	3 - 2	11986.233
4 (1, 3) - 3 (0, 3)	5 - 4	9924.254
	4 - 3	9923.851
	3 - 2	9924.366
5 (0, 5) - 4 (1, 4)	6 - 5	9653.000
	5 - 4	9652.810
	4 - 3	9653.055
5 (1, 5) - 4 (0, 4)	6 - 5	10913.892
	5 - 4	10914.168
	4 - 3	10913.842
6 (0, 6) - 5 (1, 5)	7 - 6	11816.552
	6 - 5	11816.416
	5 - 4	11816.591
6 (1, 6) - 5 (0, 5)	7 - 6	12801.450
	6 - 5	12801.681
	5 - 4	12801.420
7 (1, 7) - 6 (0, 6)	8 - 7	14692.268
	7 - 6	14692.453
	6 - 5	14692.249

Table S2. Measured transition frequencies (ν, MHz) and, in parethesis, observed – calculated values ($\Delta\nu$, kHz, rounded to the unit) for the two observed conformers of Glycidol dimer Table: Experimental rotational frequencies of anisole···$^{15}NH_3$.

J"(K_{-1}",K_1") - J'(K_{-1}',K_1')	ν / MHz
2(2, 1)- 1(1, 0)	7246.193
2(2, 0)- 1(1, 1)	7352.431
3(1, 3)- 2(0, 2)	6958.303
3(2, 2)- 2(1, 1)	9213.156
3(2, 1)- 2(1, 2)	9545.619
3(3, 1)- 2(2, 0)	11467.927
3(3, 0)- 2(2, 1)	11475.232
3(1, 2)- 2(0, 2)	7553.407
4(0, 4)- 3(1, 3)	7409.882
4(1, 4)- 3(0, 3)	8840.658
4(2, 3)- 3(1, 2)	11129.515
4(2, 2)- 3(1, 3)	11827.300
4(3, 2)- 3(2, 1)	13519.367
4(3, 1)- 3(2, 2)	13556.274
4(1, 3)- 3(0, 3)	9830.806
5(0, 5)- 4(1, 4)	9557.108
5(1, 5)- 4(0, 4)	10699.112
5(2, 4)- 4(1, 3)	12996.503
5(3, 3)- 4(2, 2)	15543.819
5(3, 2)- 4(2, 3)	15655.077
5(1, 4)- 4(0, 4)	12178.882
6(0, 6)- 5(1, 5)	11684.872
6(1, 6)- 5(0, 5)	12550.040
7(1, 7)- 6(0, 6)	14408.417
8(0, 8)- 7(1, 7)	15851.639
8(1, 8)- 7(0, 7)	16284.109

Scheme S1. Overview of the predicted structures and dissociation energies (kJ mol^{-1}) for the most stable conformers of anisole···NH_3 as obtained with different calculation methods. In bold the nick names used in the various calculations for the various conformers.

MM (Ref. 15)	B3LYP/6-311++G** (Ref. 15)	MP2/6-311+G(d,p) (Ref. 16)	Orient (this work)	$MP2_{CP}$(full)6-311++G** (this work)
a) Non-planar forms				
				
AA1: 16.18			**I**: 15.98 (11.09)[a]	
				
AA2: 15.84	**AA-I**: 6.84	**H···π**: 13.03[b] (6.59)[a]		**I**: 12.80 (9.02)[a]
				
AA3: 15.48			**IV**: 14.11 (8.44)[a]	
b) Planar forms				
				
AA4: 13.56	**AA-II**: 7.87	**NH··O**: 10.91[c] (6.66)[a]	**II**: 15.25 (9.33)[a]	**II**: 10.96 (6.49)[a]
				
AA5: 12.51	**AA-III**: 5.65	**H··N··H**: 8.56[c] (5.09)[a]	**V**: 12.98 (9.64)[a]	**V**: 8.93 (6.56)[a]
				
			III: 15.15 (9.63)[a]	**III**: 11.82 (7.52)[a]

[a] Harmonic zero point corrected dissociation energies.
[b] Value from the $MP2_{CP}$ optimized structure..
[c] BSSE corrected dissociation energies.