Erratum: "Resonance Raman intensity analysis of a dicyanovinyl-azaadamantane: Mode-specific reorganization energies for charge-transfer and locally-excited states" [J. Chem. Phys. 109, 10958 (1998)]

Mark Lilichenko and Anne Myers Kelley

Articles you may be interested in

A charge-transfer surface enhanced Raman scattering model from time-dependent density functional theory calculations on a Ag 10 -pyridine complex
J. Chem. Phys. **132**, 214707 (2010); 10.1063/1.3431210

Photoinduced charge-transfer process in rubidium manganese hexacyanoferrate probed by Raman spectroscopy
J. Chem. Phys. **131**, 154505 (2009); 10.1063/1.3245863

Resonance hyper-Raman excitation profiles of a donor-acceptor substituted distyrylbenzene: One-photon and two-photon states
J. Chem. Phys. **122**, 184508 (2005); 10.1063/1.1891708

Intramolecular vibrational energy redistribution and intermolecular energy transfer in the (d,d) excited state of nickel octaethylporphyrin
J. Chem. Phys. **111**, 8950 (1999); 10.1063/1.480253

Resonance Raman intensity analysis of a dicyanovinyl-azaadamantane: Mode-specific reorganization energies for charge-transfer and locally-excited states
J. Chem. Phys. **109**, 10958 (1998); 10.1063/1.477792

LETTERS TO THE EDITOR

The Letters to the Editor section is divided into three categories entitled Notes, Comments, and Errata. Letters to the Editor are limited to one and three-fourths journal pages as described in the Announcement in the 1 July 1999 issue.

ERRATA

Erratum: ''Resonance Raman intensity analysis of a dicyanovinyl-azaadamantane: Mode-specific reorganization energies for charge-transfer and locally-excited states'' [J. Chem. Phys. 109, 10958 (1998)]

Mark Lilichenko[a] and Anne Myers Kelley[a),b)]
Department of Chemistry and Center for Photoinduced Charge Transfer, University of Rochester, Rochester, New York 14627-0216

[S0021-9606(99)01429-4]

Due to misinterpretation of the normal mode coefficients produced by GAUSSIAN 94, an error was made in the conversion from dimensionless normal mode displacements to bond length and bond angle changes in the title paper.[1] Results reported in

TABLE IV. Ground to CT state equilibrium geometry changes (Å and degrees) of AAM.

Internal coordinate	Ground state equilibrium value (from RHF/6-31G* calculation)	Two most probable sets of geometry changes on CT excitation[a] (from resonance Raman analysis)		Internal coordinate	Ground state equilibrium value (from RHF/6-31G* calculation)	Two most probable sets of geometry changes on CT excitation[a] (from resonance Raman analysis)	
$N-C_1$	1.461	−0.0065	−0.0016	$C_9-C_{10}-C_{11}$	122.2	−0.36	−0.40
$N-C_2$	1.454	−0.0217	−0.0246	$C_{11}-C_{10}-C_{12}$	115.6	0.74	0.82
C_1-C_6	1.537	0.0075	0.0091	$C_{10}{=}C_9-C_7$	123.9	−2.04	−1.62
C_2-C_7	1.548	0.0167	0.0211	''in-plane''	179.8	0.05	0.09
C_4-C_6	1.536	0.0126	0.0114	$C_{10}-C_{11}{\equiv}N$ bend			
C_4-C_7	1.545	0.0026	0.0055	''out-of-plane''	179.1	−1.78	−2.06
C_7-C_9	1.509	0.0274	0.0253	$C_{10}-C_{11}{\equiv}N$ bend			
$C_{10}-C_{11}$	1.443	−0.0082	−0.0065	$(C_7,C_8)-C_9{=}C_{10}$	−0.6	7.37	6.72
$C_9{=}C_{10}$	1.341	0.0415	0.0435	(''out-of-plane'' deform.)			
$C_{11}{\equiv}N$	1.136	0.0105	0.0105	$C_9{=}C_{10}-(C_{11},C_{12})$	−0.2	5.85	5.75
C_1-N-C_2	110.5	1.70	2.60	(''out-of-plane'' deform.)			
C_2-N-C_3	109.9	3.82	1.15	C_1-C_6-H	110.0	3.51	3.47
$N-C_1-C_6$	111.1	−3.02	−2.46	C_2-C_7-H	110.4	1.15	0.79
$N-C_2-C_7$	111.2	−0.78	−0.64	C_4-C_6-H	110.0	−2.34	−2.06
$N-C_1-H$	108.5	0.26	0.07	C_4-C_7-H	110.7	−1.45	−1.83
$N-C_2-H'$	109.1	−1.02	−1.57	C_6-C_1-H	110.7	1.06	0.95
$N-C_2-H''$	109.2	−0.66	0.22	C_6-C_4-H'	110.8	−3.17	−3.43
$C_1-C_6-C_4$	108.8	0.12	0.44	C_6-C_4-H''	110.7	3.17	3.60
$C_2-C_7-C_4$	108.5	−0.85	0.68	C_7-C_2-H'	110.6	1.31	0.61
$C_4-C_6-C_5$	109.1	0.95	−0.21	C_7-C_2-H''	109.3	1.61	1.87
$C_6-C_4-C_7$	109.1	0.90	0.87	C_7-C_4-H'	110.4	1.74	1.24
$C_7-C_9-C_8$	112.2	4.18	3.34	C_7-C_4-H''	108.8	−2.08	−1.77
$C_9-C_7-C_2$	107.5	−4.26	−4.73	C_9-C_7-H	111.3	5.23	5.29
$C_9-C_7-C_4$	108.4	−0.04	−0.39				

[a]Geometry changes are given as excited state geometry minus ground state geometry.

[a)]Current address: Department of Chemistry, Kansas State University, Willard Hall, Manhattan, KS 66506-3701.
[b)]Author to whom correspondence should be addressed. Electronic mail: amkelley@ksu.edu

TABLE V. The early time dynamics of AAM following CT excitation (Å and degrees).[a]

Internal coordinate	Internal coordinate displacements at various times			Internal coordinate	Internal coordinate displacements at various times		
	5 fs	10 fs	15 fs		5 fs	10 fs	15 fs
$N–C_1$	0.0014	0.0026	−0.0022	$C_9–C_{10}–C_{11}$	−0.57	−1.07	−0.42
$N–C_2$	−0.0084	−0.0275	−0.0423	$C_{11}–C_{10}–C_{12}$	1.14	2.16	0.87
$C_1–C_6$	0.0052	0.0147	0.0176	$C_{10}=C_9–C_7$	−0.99	−2.45	−2.53
$C_2–C_7$	0.0097	0.0291	0.0396	''in-plane''	0.56	0.99	0.14
$C_4–C_6$	0.0014	0.0065	0.0159	$C_{10}–C_{11}≡N$ bend			
$C_4–C_7$	−0.0001	−0.0019	−0.005	''out-of-plane''	−0.46	−1.63	−2.96
$C_7–C_9$	−0.0052	0.0022	0.0417	$C_{10}–C_{11}≡N$ bend			
$C_{10}–C_{11}$	−0.0177	−0.0222	−0.0026	$(C_7,C_8)–C_9=C_{10}$	1.88	6.45	11.08
$C_9=C_{10}$	0.0366	0.0749	0.0422	(''out-of-plane'' deform.)			
$C_{11}≡N$	0.0160	0.0123	−0.0001	$C_9=C_{10}–(C_{11},C_{12})$	1.37	4.83	8.69
$C_1–N–C_2$	0.29	1.11	2.22	(''out-of-plane'' deform.)			
$C_2–N–C_3$	0.59	2.09	3.86	$C_1–C_6–H$	1.48	4.53	6.31
$N–C_1–C_6$	−0.66	−2.26	−3.98	$C_2–C_7–H$	−0.53	−0.70	1.13
$N–C_2–C_7$	0.11	0.25	0.00	$C_4–C_6–H$	−0.90	−2.84	−4.18
$N–C_1–H$	0.12	0.27	0.15	$C_4–C_7–H$	−1.39	−3.41	−2.95
$N–C_2–H'$	−0.62	−1.66	−1.81	$C_6–C_1–H$	0.10	0.55	1.47
$N–C_2–H''$	−0.01	−0.20	−0.85	$C_6–C_4–H'$	−1.47	−4.35	−5.72
$C_1–C_6–C_4$	−0.01	0.08	0.37	$C_6–C_4–H''$	1.84	5.26	6.30
$C_2–C_7–C_4$	−0.38	−0.96	−0.98	$C_7–C_2–H'$	0.70	1.92	2.12
$C_4–C_6–C_5$	0.35	1.03	1.37	$C_7–C_2–H''$	0.08	0.37	1.25
$C_6–C_4–C_7$	0.24	0.77	1.19	$C_7–C_4–H'$	0.91	2.74	3.64
$C_7–C_9–C_8$	2.00	4.99	5.20	$C_7–C_4–H''$	−1.24	−3.69	−4.60
$C_9–C_7–C_2$	−1.44	−4.49	−6.85	$C_9–C_7–H$	3.69	9.23	8.82
$C_9–C_7–C_4$	−0.04	0.11	0.51				

[a]The signs of the displacements correspond to the first of the two geometries given in Table IV.

terms of dimensionless displacements or reorganization energies are not affected, and the qualitative conclusions regarding the geometry changes in the charge-transfer and locally-excited states remain valid, but the values for the bond length and bond angle changes reported were generally too large by factors of two to three. Here we present corrected versions of Tables IV and V. Table IV lists only the ''same'' two geometries (same combinations of signs of the dimensionless displacements) that were found in the original paper, although the corrected calculation finds four additional possible geometries that satisfy theselection criteria employed. Also, the change in C=C bond length in the locally excited state if only the 1585 cm^{-1} mode is assumed to contribute to this stretching coordinate, originally reported as 0.20 Å, should instead be 0.072 Å, and the possible range of C=C bond length changes in the LE state when all possible sign combinations of the deltas are considered, originally reported as 0.19 to 0.21 Å, should instead be 0.067 to 0.077 Å.

Figures 6 and 7 of the original paper, in which the geometry changes were deliberately exaggerated, remain qualitatively correct, but the actual degree of exaggeration is greater than originally reported.

[1]M. Lilichenko, D. Tittelbach-Helmrich, J. W. Verhoeven, I. R. Gould, and A. B. Myers, J. Chem. Phys. **109**, 10958 (1998).