Supplementary Materials

Cyclohexane Vibronic States: A Combined VUV Spectroscopy and Theoretical Study

Edvaldo Bandeira [1], Alessandra S. Barbosa [1], Nykola C. Jones [2], Søren V. Hoffmann [2], Márcio H. F. Bettega [1,*] and Paulo Limão-Vieira [1,3,*]

[1] Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044, Curitiba 81531-980, PR, Brazil
[2] ISA, Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, DK-8000 Aarhus C, Denmark
[3] Atomic and Molecular Collisions Laboratory, Centre of Physics and Technological Research (CEFITEC), Department of Physics, NOVA School of Science and Technology, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal
* Correspondence: bettega@fisica.ufpr.br (M.H.F.B.); plimaovieira@fct.unl.pt (P.L.-V.); Tel.: +55-41-3361-3002 (M.H.F.B.); +351-21-294-78-59 (P.L.-V.)

Figure captions

Figure S1. Electronic configuration, cartesian coordinates and neutral *chair* ground-state geometry of cyclohexane obtained at the DFT/CAMB3LYP/aug-cc-pVTZ level of theory. Bond lengths are in Å and bond angles in (°). The plot was obtained with MacMolPlt graphical interface [1].

Figure S2. Cartesian coordinates and cationic *boat* ground-state geometry cyclohexane obtained at the DFT/CAMB3LYP/aug-cc-pVTZ level of theory. Bond lengths are in Å and bond angles in (°). The plot was obtained with MacMolPlt graphical interface [1].

Figure S3. Representation of a selection of cyclohexane molecular orbitals computed at the DFT/CAMB3LYP/aug-cc-pVTZ level of theory. The plots were obtained with MacMolPlt graphical interface [1].

Figure S4. Potential energy curves for the ground and the ten lowest-lying singlet excited states of cyclohexane, following the CCC bending/CC torsion $v'_{24}(e_g)$ and for C–C stretching, $v'_{27/28}(e_g)$ modes (in a_0 units). The calculations were performed at the TD-DFT/CAMB3LYP/aug-cc-pVTZ level of theory in the C_1 symmetry group. See text for details.

Table caption

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Table S2. The calculated vertical excitation energies and oscillator strengths (TD-DFT/CAMB3LYP/aug-cc-pVTZ) of *chair* cyclohexane (energies in eV). See text for details.

Table S3. Harmonic frequencies computed at the DFT/CAMB3LYP/ aug-cc-pVTZ level of theory for *chair* cyclohexane neutral electronic ground-state, compared with experimental data.

Table S4. Harmonic frequencies computed at the DFT/CAMB3LYP/aug-cc-pVTZ level of theory for cationic *boat-axial* ground-state cyclohexane.

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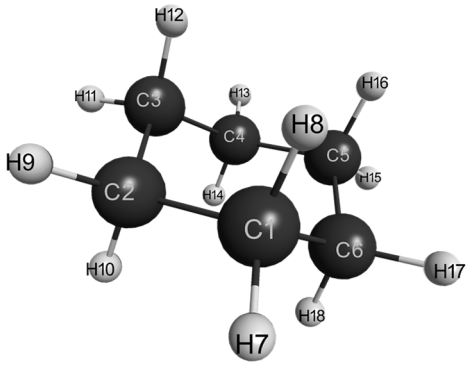
Electronic configuration of $\tilde{X}\ ^1A_{1g}$ state:

core orbitals: $(1a_{1g})^2\ (1e_u)^4\ (1e_g)^4\ (1a_{2u})^2\ (2a_{1g})^2\ (2e_u)^4\ (2e_g)^4$

valence orbitals: $(2a_{2u})^2\ (3a_{1g})^2\ (3a_{2u})^2\ (3e_g)^4\ (3e_u)^4\ (1a_{1u})^2\ (4e_u)^4\ (4a_{1g})^2\ (4e_g)^4$

unoccupied orbitals: $(5a_{1g})\ (4a_{2u})\ (5e_u)\ (5e_g)\ (6a_{1g})\ (6e_g)\ (5a_{2u})\ (6e_u)\ (7e_u)\ (6a_{2u})\ (7a_{1g})\ (2a_{1u})\ (7a_{2u})\ (8e_u)\ (8e_g)\ (8a_{1g})$

Cartesian coordinates of all atoms				
Atom	*x* (Å)	*y* (Å)	*z* (Å)	
C1	1.26040208	0.7276935	0.22866955	
C2	1.26040208	-0.7276935	-0.22866955	
C3	0	-1.455387	0.22866955	
C4	-1.26040208	-0.7276935	-0.22866955	
C5	-1.26040208	0.7276935	0.22866955	
C6	0	1.455387	-0.22866955	
H7	2.14908433	1.24077439	-0.14190041	
H8	1.31544864	0.75947464	1.32092595	
H9	2.14908433	-1.24077439	0.14190041	
H10	1.31544864	-0.75947464	-1.32092595	
H11	0	-2.48154879	-0.14190041	
H12	0	-1.51894927	1.32092595	
H13	-2.14908433	-1.24077439	0.14190041	
H14	-1.31544864	-0.75947464	-1.32092595	
H15	-2.14908433	1.24077439	-0.14190041	
H16	-1.31544864	0.75947464	1.32092595	
H17	0	2.48154879	0.14190041	
H18	0	1.51894927	-1.32092595	



bond length (Å)		angle (°)	
C1 – C2	1.5256	C3 – C2 – C1	111.42
C2 – C3	1.5256	C4 – C3 – C2	111.42
C3 – C4	1.5256	C5 – C4 – C3	111.42
C4 – C5	1.5256	C6 – C5 – C4	111.42
C5 – C6	1.5256	H7 – C1 – C2	110.29
H7 – C1	1.0910	H8 – C1 – H7	106.53
H8 – C1	1.0941	H9 – C2 – C1	110.29
H9 – C2	1.0910	H10 – C2 – H9	106.53
H10 – C2	1.0941	H11 – C3 – C2	110.29
H11 – C3	1.0910	H12 – C3 – H11	106.53
H12 – C3	1.0941	H13 – C4 – C3	110.29
H13 – C4	1.0910	H14 – C4 – H13	106.53
H14 – C4	1.0941	H15 – C5 – C4	110.29
H15 – C5	1.0910	H16 – C5 – H15	106.53
H16 – C5	1.0941	H17 – C6 – C1	110.29
H17 – C6	1.0910	H18 – C6 – H17	106.53
H18 – C6	1.0941		

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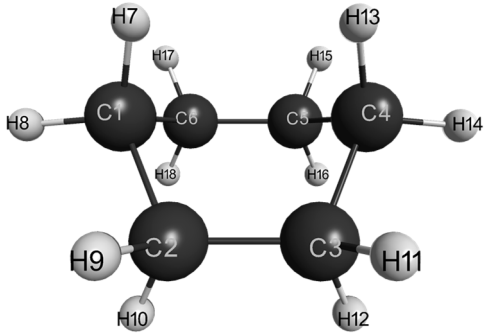
Cartesian coordinates of all atoms				
Atom	*x* (Å)	*y* (Å)	*z* (Å)	
C1	-1.37436247	0.00000183	0.41120121	
C2	-0.74503022	-1.22804642	-0.32027557	
C3	0.74501783	-1.22804976	-0.32024953	
C4	1.37437475	0.00000046	0.41118026	
C5	0.74501675	1.22804832	-0.32024664	
C6	-0.74503195	1.22804654	-0.32027662	
H7	-1.12838876	0.00000006	1.46799088	
H8	-2.45441985	-0.00000055	0.30618018	
H9	-1.1488601	-2.04769325	0.30080441	
H10	-1.1645999	-1.32290149	-1.31751633	
H11	1.14886093	-2.04770756	0.3007926	
H12	1.16460061	-1.32290125	-1.31749403	
H13	1.12839758	-0.00000061	1.46797955	
H14	2.45442939	-0.00000207	0.3061839	
H15	1.14886069	2.04770851	0.30079159	
H16	1.16459584	1.32289934	-1.31749272	
H17	-1.14886069	2.04769421	0.30080423	
H18	-1.16460037	1.32290339	-1.31751728	



bond length (Å)		angle (°)	
C1 – C2	1.5618	C3 – C2 – C1	113.76
C2 – C3	1.4901	C4 – C3 – C2	113.77
C3 – C4	1.5618	C5 – C4 – C3	103.68
C4 – C5	1.5618	C6 – C5 – C4	113.77
C5 – C6	1.4901	H7 – C1 – C2	111.40
H7 – C1	1.0850	H8 – C1 – H7	108.66
H8 – C1	1.0852	H9 – C2 – C1	99.95

H9 – C2	1.1048	H10 – C2 – H9	108.07
H10 – C2	1.0861	H11 – C3 – C4	99.95
H11 – C3	1.1048	H12 – C3 – H11	108.07
H12 – C3	1.0861	H13 – C4 – C5	111.39
H13 – C4	1.0851	H14 – C4 – H13	108.66
H14 – C4	1.0852	H15 – C5 – C4	99.95
H15 – C5	1.1048	H16 – C5 – H15	108.07
H16 – C5	1.0861	H17 – C6 – C1	99.95
H17 – C6	1.1048	H18 – C6 – H17	108.07
H18 – C6	1.0861		

Figure S3. Representation of a selection of cyclohexane molecular orbitals computed at the DFT/CAMB3LYP/aug-cc-pVTZ level of theory. The plots were obtained with MacMolPlt graphical interface [1].

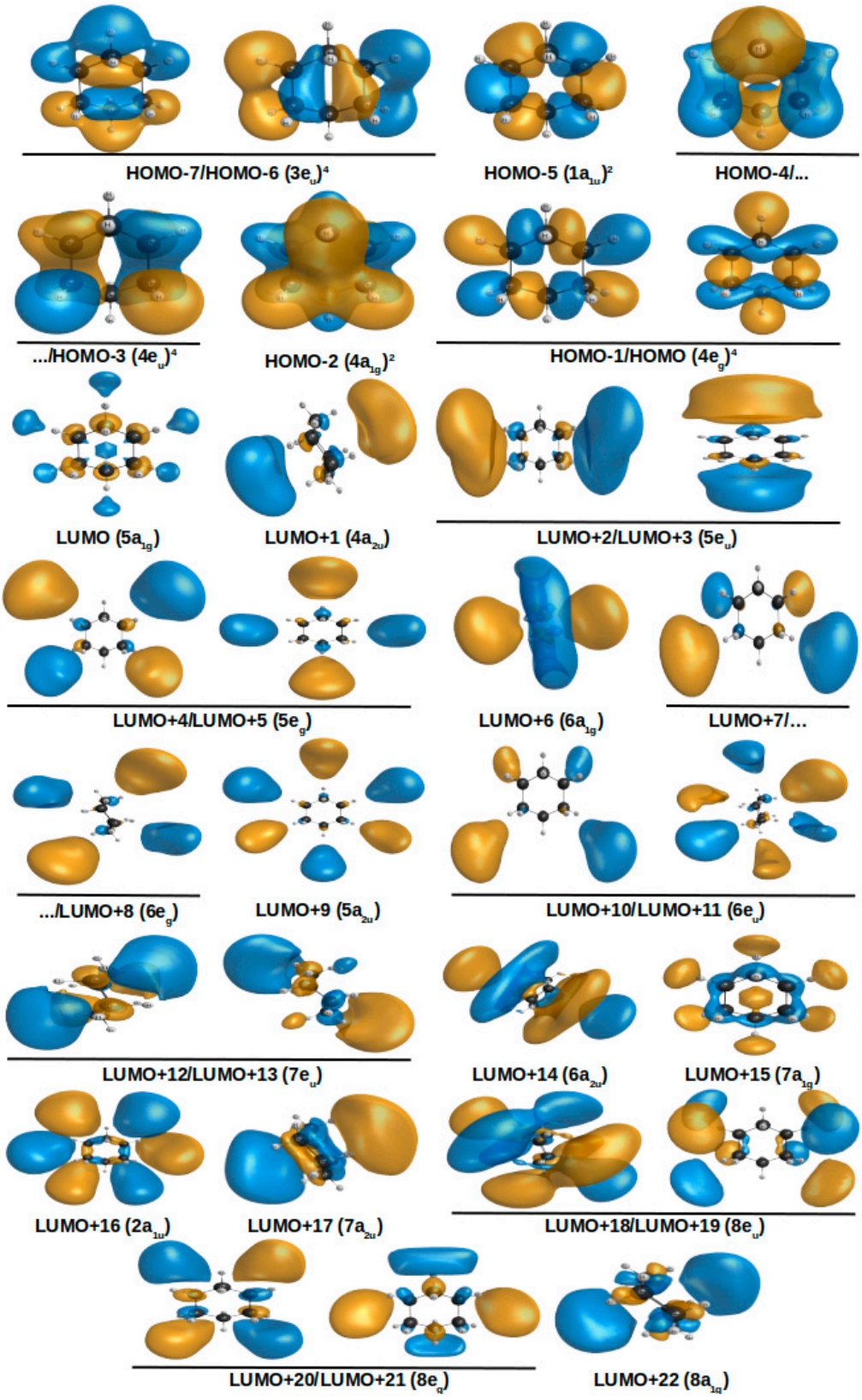


Figure S4. Potential energy curves for the ground and the ten lowest-lying singlet excited states of cyclohexane, following the C–C stretching, $v_5'(a_{1g})$ and CCC bending/CC torsion $v_{24}'(e_g)$ modes (in a_0 units). The calculations were performed at the TD-DFT/CAMB3LYP/aug-cc-pVTZ level of theory in the C_1 symmetry group. See text for details.

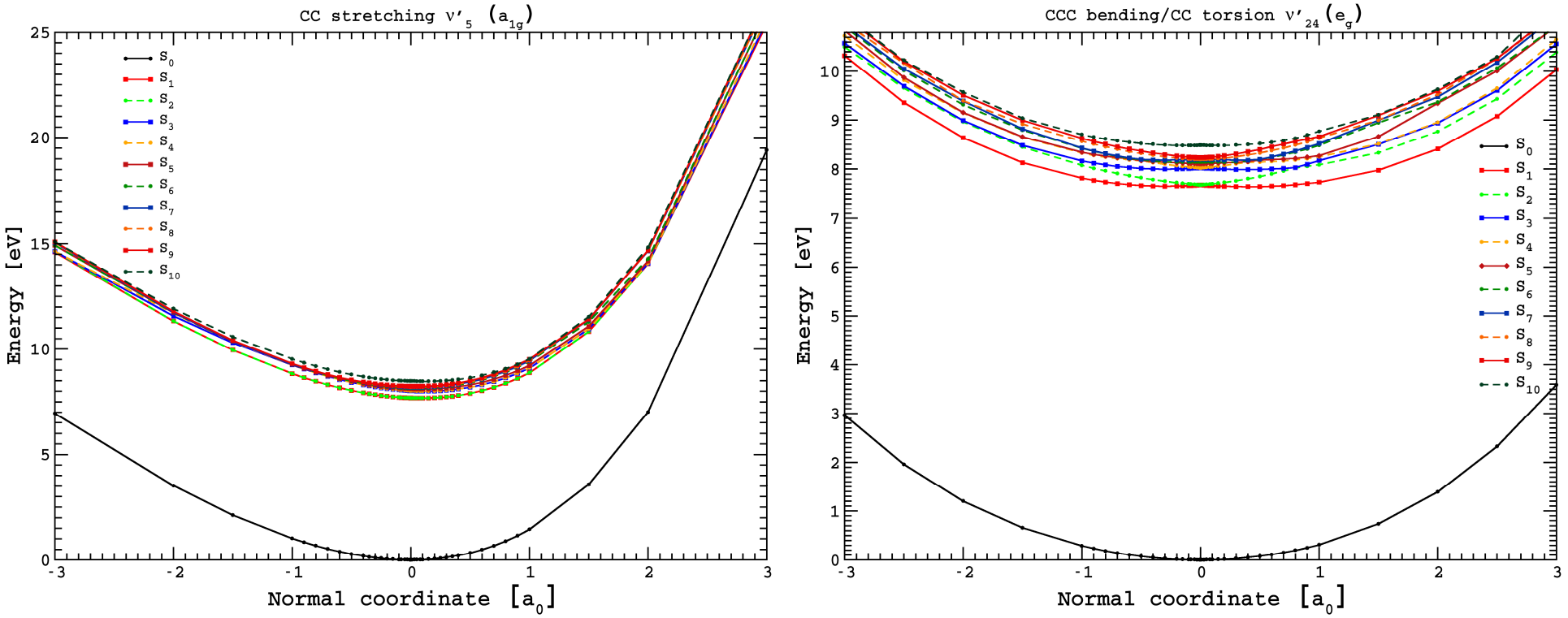


Table S1. Total energy values with zero-point correction computed at the DFT/CAMB3LYP/ aug-cc-pVTZ level of theory for cyclohexane conformers in the neutral ground-state and first excited state. Also included is the energy difference ΔE with respect to the energy of the most stable conformer.

$\tilde{X}\ ^1A_{1g}$		
conformer	Energy (Hartree)	ΔE (eV)
chair	-235.644497	–
twist-boat	-235.634694	0.27
$\tilde{X}\ ^2E_g$		
boat-axial	-235.2582303	10.51

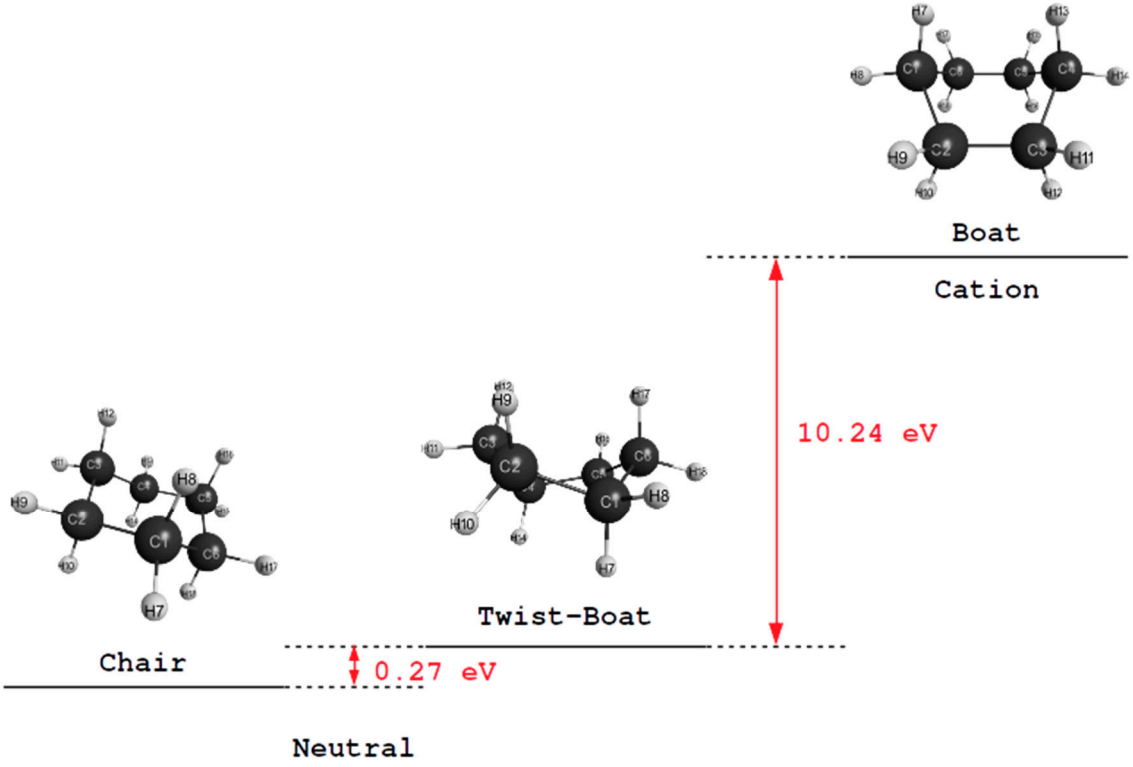


Table S2. The calculated vertical excitation energies and oscillator strengths (TD-DFT/CAMB3LYP/aug-cc-pVTZ) of *chair* cyclohexane (energies in eV). See text for details.

cyclohexane				
State (C_{2h})	State (D_{3d})	E (eV)	f_L	Dominant excitations
A_g	E_g	7.681	0	HOMO->LUMO (91%)
B_g	E_g	7.681	0	H-1->LUMO (91%)
B_u	E_u	8.025	0.000171	HOMO->L+1 (90%)
A_u	E_u	8.026	0.000172	H-1->L+1 (90%)
A_g	A_{1g}	8.112	0	H-2->LUMO (83%)
B_u	A_{2u}	8.147	0.002014	H-1->L+2 (44%), HOMO->L+3 (44%)
A_u	E_u	8.198	0.034207	HOMO->L+2 (43%), H-1->L+3 (43%)
B_u	E_u	8.198	0.034198	H-1->L+2 (43%), HOMO->L+3 (43%)
A_u	A_{1u}	8.234	0	HOMO->L+2 (43%), H-1->L+3 (44%)
A_u	E_u	8.482	0.003019	H-3->LUMO (30%), H-2->L+2 (54%)
B_u	E_u	8.482	0.003035	H-4->LUMO (30%), H-2->L+3 (54%)
B_u	A_{2u}	8.487	0.221001	H-2->L+1 (90%)
B_g	A_{2g}	8.804	0	HOMO->L+4 (44%), H-1->L+5 (42%)
A_g	E_g	8.808	0	H-1->L+4 (41%), HOMO->L+5 (41%)
B_g	E_g	8.808	0	HOMO->L+4 (40%), H-1->L+5 (42%)
A_g	A_{1g}	8.870	0	H-1->L+4 (44%), HOMO->L+5 (44%)
A_g	E_g	8.946	0	HOMO->L+6 (82%)
B_g	E_g	8.946	0	H-1->L+6 (82%)
A_g	A_{1g}	8.964	0	H-1->L+7 (46%), HOMO->L+8 (46%)
B_g	E_g	8.990	0	HOMO->L+7 (44%), H-1->L+8 (44%)

A_g	E_g	8.990	0	H-1->L+7 (44%), HOMO->L+8 (44%)
B_g	A_{2g}	9.010	0	HOMO->L+7 (44%), H-1->L+8 (44%)
B_g	E_g	9.020	0	H-3->L+1 (50%), H-2->L+7 (16%)
A_g	E_g	9.020	0	H-4->L+1 (50%), H-2->L+8 (16%)
A_g	E_g	9.135	0	H-4->L+1 (16%), H-3->L+2 (13%), H-4->L+3 (13%), H-2->L+5 (39%)
B_g	E_g	9.136	0	H-3->L+1 (16%), H-4->L+2 (13%), H-3->L+3 (13%), H-2->L+4 (39%)
A_u	E_u	9.137	0.003653	H-3->LUMO (59%), H-2->L+2 (32%)
B_u	E_u	9.137	0.003655	H-4->LUMO (59%), H-2->L+3 (32%)
A_g	A_{1g}	9.331	0	H-3->L+2 (14%), H-4->L+3 (14%), H-2->L+6 (61%)
B_g	A_{2g}	9.501	0	H-4->L+2 (44%), H-3->L+3 (44%)
B_g	E_g	9.589	0	H-3->L+1 (22%), H-2->L+7 (70%)
A_g	E_g	9.589	0	H-4->L+1 (22%), H-2->L+8 (70%)
A_g	A_{1g}	9.635	0	H-3->L+2 (27%), H-4->L+3 (27%), H-2->L+6 (28%)
B_u	E_u	9.677	0.094041	HOMO->L+9 (83%)
A_u	E_u	9.677	0.094079	H-1->L+9 (83%)
B_g	E_g	9.705	0	H-4->L+2 (24%), H-3->L+3 (25%), H-2->L+4 (41%)
A_g	E_g	9.706	0	H-3->L+2 (24%), H-4->L+3 (24%), H-2->L+5 (41%)
B_u	A_{2u}	9.748	0.000047	H-1->L+10 (34%), HOMO->L+11 (34%)
A_u	A_{1u}	9.760	0	H-5->LUMO (15%), HOMO->L+10 (27%), H-1->L+11 (24%)
A_u	E_u	9.766	0.000238	HOMO->L+10 (30%), H-1->L+11 (33%)
B_u	E_u	9.766	0.000235	H-1->L+10 (31%), HOMO->L+11 (32%)
A_u	A_{1u}	9.893	0	H-5->LUMO (51%), HOMO->L+10 (10%), H-1->L+11 (10%)
B_u	A_{2u}	9.905	0.047456	H-3->L+4 (28%), H-4->L+5 (28%), H-2->L+9 (29%)
A_u	A_{1u}	9.959	0	H-5->LUMO (12%), H-4->L+4 (29%), H-3->L+5 (29%), H-2->L+16 (10%)
B_u	E_u	9.978	0.003086	H-4->L+6 (38%), H-2->L+11 (18%)
A_u	E_u	9.978	0.002958	H-3->L+6 (38%), H-2->L+10 (18%)

A_u	E_u	10.014	0.106166	H-6->LUMO (28%), H-1->L+14 (33%), H-1->L+17 (13%)
B_u	E_u	10.014	0.104961	H-7->LUMO (28%), HOMO->L+14 (35%), HOMO->L+17 (13%)
B_u	E_u	10.039	0.030083	H-7->LUMO (17%), H-4->L+6 (10%), HOMO->L+14 (11%), HOMO->L+17 (11%)
A_u	E_u	10.040	0.028772	H-6->LUMO (17%), H-1->L+14 (15%), H-1->L+17 (12%)
B_u	A_{2u}	10.060	0.009169	H-1->L+12 (18%), HOMO->L+13 (18%)
B_u	A_{2u}	10.091	0.022573	H-3->L+7 (18%), H-4->L+8 (29%), H-2->L+14 (11%)
A_u	E_u	10.094	0.016806	H-4->L+7 (31%), H-3->L+8 (31%)
B_u	E_u	10.094	0.017719	H-3->L+7 (36%), H-4->L+8 (26%)
A_u	A_{1u}	10.123	0.000391	HOMO->L+12 (27%), H-1->L+13 (21%), H-1->L+18 (10%), HOMO->L+19 (13%)
A_u	E_u	10.129	0.029875	H-1->L+13 (13%), HOMO->L+16 (45%)
B_u	E_u	10.129	0.029374	H-1->L+16 (45%)
B_g	E_g	10.157	0	H-1->L+15 (78%)
A_g	E_g	10.157	0	HOMO->L+15 (78%)
A_u	Eu	10.165	0.000395	H-4->L+4 (39%), H-3->L+5 (39%)
B_u	E_u	10.165	0.000358	H-3->L+4 (39%), H-4->L+5 (39%)
B_u	E_u	10.170	0.00553	H-7->LUMO (15%), H-1->L+16 (36%)
A_u	E_u	10.170	0.005672	H-6->LUMO (15%), HOMO->L+16 (37%)
B_g	A_{2g}	10.184	0	H-5->L+1 (82%)
A_u	E_u	10.217	0.011131	H-1->L+14 (26%), H-1->L+17 (51%)
B_u	E_u	10.217	0.011318	HOMO->L+14 (26%), HOMO->L+17 (50%)
A_u	A_{1u}	10.273	0	H-4->L+7 (45%), H-3->L+8 (45%)
B_g	E_g	10.348	0	H-6->L+1 (83%)
A_g	E_g	10.348	0	H-7->L+1 (83%)
Bu	A_{2u}	10.389	0.002959	HOMO->L+18 (32%), H-1->L+19 (34%)
A_u	E_u	10.402	0.033565	H-3->L+6 (25%), H-2->L+10 (46%), H-2->L+12 (10%)
B_u	E_u	10.402	0.033467	H-4->L+6 (25%), H-2->L+11 (46%), H-2->L+13 (10%)

B_g	E_g	10.410	0	H-5->L+3 (61%)
A_g	E_g	10.410	0	H-5->L+2 (60%)
B_u	A_{2u}	10.443	0.006024	H-3->L+4 (14%), H-4->L+5 (14%), H-2->L+9 (47%)
A_g	E_g	10.461	0	H-6->L+2 (23%), H-7->L+3 (24%), H-1->L+20 (14%), HOMO->L+21 (13%)
B_g	E_g	10.462	0	HOMO->L+20 (34%), H-1->L+21 (31%)
A_u	E_u	10.481	0.002121	HOMO->L+12 (13%), H-1->L+18 (21%), HOMO->L+19 (36%)
B_u	E_u	10.481	0.002179	H-1->L+12 (10%), HOMO->L+13 (11%), HOMO->L+18 (29%), H-1->L+19 (28%)
A_u	A_{1u}	10.487	0.000039	H-1->L+13 (15%), H-1->L+18 (37%), HOMO->L+19 (22%)
A_g	E_g	10.549	0	H-6->L+2 (13%), H-7->L+3 (11%), H-1->L+20 (27%), HOMO->L+21 (26%)
B_g	E_g	10.550	0	H-7->L+2 (12%), H-6->L+3 (13%), HOMO->L+20 (25%), H-1->L+21 (27%)
A_g	E_g	10.593	0	H-6->L+2 (26%), H-5->L+2 (13%), H-7->L+3 (27%), HOMO->L+22 (12%)
B_g	E_g	10.594	0	H-7->L+2 (26%), H-6->L+3 (25%), H-5->L+3 (13%), H-1->L+22 (12%)
A_g	A_{1g}	10.610	0	H-2->L+15 (70%)
A_g	A_{1g}	10.639	0	H-6->L+2 (15%), H-7->L+3 (15%), H-1->L+20 (27%), HOMO->L+21 (30%)
A_u	E_u	10.646	0.00459	H-2->L+10 (19%), H-2->L+12 (53%)
B_u	E_u	10.649	0.004624	H-2->L+11 (18%), H-2->L+13 (53%)
B_u	A_{2u}	10.654	0.004345	H-2->L+9 (10%), H-2->L+14 (67%)
B_g	A_{2g}	10.729	0	H-7->L+2 (39%), H-6->L+3 (38%)
B_u	A_{2u}	10.751	0.173676	H-2->L+17 (87%)
A_g	E_g	10.756	0	HOMO->L+22 (68%)
B_g	E_g	10.756	0	H-1->L+22 (67%)
A_u	A_{1u}	10.854	0	H-2->L+16 (75%)
B_g	E_g	10.877	0	H-3->L+9 (30%), H-2->L+20 (27%)
A_g	E_g	10.878	0	H-4->L+9 (31%), H-2->L+21 (26%)
A_g	E_g	10.907	0	H-4->L+9 (30%), H-3->L+10 (13%), H-4->L+11 (13%)
B_g	E_g	10.907	0	H-3->L+9 (30%), H-4->L+10 (13%), H-3->L+11 (13%), H-3->L+14 (10%)

A_g	A_{1g}	10.937	0	H-1->L+23 (42%), HOMO->L+24 (41%)
A_u	A_{1u}	10.960	0.017794	H-2->L+19 (70%)

Table S3. Harmonic frequencies computed at the DFT/CAMB3LYP/ aug-cc-pVTZ level of theory for *chair* cyclohexane neutral electronic ground-state, compared with experimental data.

$\tilde{X}\ ^1A_{1g}$								
this work		mode	C_{2h}	mode	D_{3d}	*	Exp. [2]	Assignment
cm^{-1}	eV					eV	cm^{-1}	
3079.11	0.3817	1	A_g	1	A_{1g}	0.3642	2930	CH_2 s-stretching
3024.79	0.3750	2	A_g	2	A_{1g}	0.3578	2852	CH_2 s-stretching
1521.12	0.1886	3	A_g	3	A_{1g}	0.1799	1465	CH_2 scissoring
1202.76	0.1491	4	A_g	4	A_{1g}	0.1423	1157	CH_2 rocking
820.87	0.1018	5	A_g	5	A_{1g}	0.0971	802	CC stretching
392.58	0.0487	6	A_g	6	A_{1g}	0.0464	383	CCC bending + CC torsion
1386.56	0.1719	7	A_u	7	A_{1u}	0.1640	1383	CH_2 twisting
1143.16	0.1417	8	A_u	8	A_{1u}	0.1352	1157	CH_2 wagging
1118.90	0.1387	9	A_u	9	A_{1u}	0.1323	1057	CC stretching + CC torsion
1364.93	0.1692	10	B_g	10	A_{2g}	0.1614	1437	CH_2 wagging
1081.29	0.1341	11	B_g	11	A_{2g}	0.1279	1090	CH_2 twisting
3084.33	0.3824	12	B_u	12	A_{2u}	0.3648	2915	CH_2 a-stretching
3032.94	0.3760	13	B_u	13	A_{2u}	0.3587	2860	CH_2 s-stretching
1506.44	0.1868	14	B_u	14	A_{2u}	0.1782	1437	CH_2 scissoring
1061.46	0.1316	15	B_u	15	A_{2u}	0.1255	1030	CH_2 rocking
539.13	0.0668	16	B_u	16	A_{2u}	0.0638	523	CCC stretching
3077.12	0.3815	17	A_g	17	E_g	0.3640	2930	CH_2 a-stretching
3077.12	0.3815	18	B_g					
3029.87	0.3756	19	A_g	18	E_g	0.3584	2897	CH_2 s-stretching
3029.87	0.3756	20	B_g					
1495.03	0.1854	21	A_g	19	E_g	0.1768	1443	CH_2 scissoring
1495.03	0.1854	22	B_g					
1395.44	0.1730	23	A_g	20	E_g	0.1650	1347	CH_2 wagging
1395.44	0.1730	24	B_g					
1305.36	0.1618	25	A_g	21	E_g	0.1544	1266	CH_2 twisting
		26	B_g					
1051.82	0.1304	27	A_g	22	E_g	0.1244	1027	CC stretching
		28	B_g					
811.39	0.1006	29	A_g	23	E_g	0.0960	785	CH_2 rocking
		30	B_g					
435.75	0.0540	31	A_g	24	E_g	0.0515	426	CCC bending + CC torsion
		32	B_g					
3075.54	0.3813	33	A_u	25	E_u	0.3638	2933	CH_2 a-stretching
		34	B_u					
3023.70	0.3749	35	A_u	26	E_u	0.3576	2863	CH_2 s-stretching
		36	B_u					
1500.91	0.1861	37	A_u	27	E_u	0.1775	1457	CH_2 scissoring
		38	B_u					
1399.99	0.1736	39	A_u	28	E_u	0.1656	1355	CH_2 wagging
		40	B_u					
1297.67	0.1609	41	A_u	29	E_u	0.1535	1261	CH_2 twisting
		42	B_u					
932.13	0.1156	43	A_u	30	E_u	0.1102	907	CH_2 rocking

		44	B_u					
882.48	0.1094	45	A_u	31	E_u	0.1044	863	CC stretching
		46	B_u					
242.99	0.0301	47	A_u	32	E_u	0.0287	284	CCC bending + CC torsion
		48	B_u					

* energy with scaling factor correction (0.954) for CAMB3LYP [3]

Table S4. Harmonic frequencies computed at the DFT/CAMB3LYP/aug-cc-pVTZ level of theory for cationic *boat-axial* ground-state cyclohexane.

$\tilde{X}\ ^2A$				
this work		*	mode	assignment
cm^{-1}	eV	eV		
3185.81	0.3950	0.3768	ν_1(a)	CH_2 s-stretching
3178.29	0.3940	0.3759	ν_2(a)	CH_2 a-stretching
3149.84	0.3905	0.3726	ν_3(a)	CH_2 s-stretching
3147.81	0.3903	0.3723	ν_4(a)	CH s-stretching
3137.03	0.3889	0.3711	ν_5(a)	CH + CH_2 s-stretching
3135.60	0.3888	0.3709	ν_6(a)	CH a-stretching
3130.25	0.3881	0.3702	ν_7(a)	CH_2 s-stretching
3117.34	0.3865	0.3687	ν_8(a)	CH_2 s-stretching
2949.26	0.3656	0.3488	ν_9(a)	CH_2 s-stretching
2909.64	0.3607	0.3442	ν_{10}(a)	CH a-stretching
2906.20	0.3603	0.3437	ν_{11}(a)	CH a-stretching
2883.37	0.3575	0.3410	ν_{12}(a)	CH a-stretching
1525.92	0.1892	0.1805	ν_{13}(a)	CH_2 scissoring
1492.66	0.1851	0.1766	ν_{14}(a)	CH_2 scissoring
1463.08	0.1814	0.1731	ν_{15}(a)	CH_2 scissoring
1462.98	0.1814	0.1730	ν_{16}(a)	CH_2 scissoring
1444.36	0.1791	0.1708	ν_{17}(a)	CH_2 scissoring
1439.32	0.1784	0.1702	ν_{18}(a)	CH_2 scissoring
1338.24	0.1659	0.1583	ν_{19}(a)	CH_2 wagging
1329.57	0.1648	0.1573	ν_{20}(a)	CH_2 wagging
1308.70	0.1623	0.1548	ν_{21}(a)	CH_2 wagging
1279.97	0.1587	0.1514	ν_{22}(a)	CH_2 wagging
1277.96	0.1584	0.1512	ν_{23}(a)	CH_2 wagging
1246.29	0.1545	0.1474	ν_{24}(a)	CH_2 twisting
1202.96	0.1491	0.1423	ν_{25}(a)	CH_2 twisting
1190.23	0.1476	0.1408	ν_{26}(a)	CH_2 wagging
1151.36	0.1427	0.1362	ν_{27}(a)	CH_2 rocking
1111.69	0.1378	0.1315	ν_{28}(a)	CC stretching + CC torsion
1105.92	0.1371	0.1308	ν_{29}(a)	CH_2 wagging
1058.61	0.1312	0.1252	ν_{30}(a)	CH_2 twisting
1009.94	0.1252	0.1195	ν_{31}(a)	CH_2 twisting
979.83	0.1215	0.1159	ν_{32}(a)	CCC deformation
947.90	0.1175	0.1121	ν_{33}(a)	CC stretching
943.17	0.1169	0.1116	ν_{34}(a)	CC stretching
903.36	0.1120	0.1069	ν_{35}(a)	CH_2 rocking
831.30	0.1031	0.0983	ν_{36}(a)	CC stretching
819.23	0.1016	0.0969	ν_{37}(a)	CC stretching
744.97	0.0924	0.0881	ν_{38}(a)	CCC deformation + CC stretching
673.68	0.0835	0.0797	ν_{39}(a)	CH_2 rocking
615.80	0.0763	0.0728	ν_{40}(a)	CC stretching
578.37	0.0717	0.0684	ν_{41}(a)	CH_2 rocking
463.23	0.0574	0.0548	ν_{42}(a)	CCC bending + CC torsion
429.70	0.0533	0.0508	ν_{43}(a)	CCC bending + CC torsion
373.80	0.0463	0.0442	ν_{44}(a)	CCC stretching + CC torsion
310.83	0.0385	0.0368	ν_{45}(a)	CCC bending + CC torsion

300.16	0.0372	0.0355	ν_{46}(a)	CCC bending + CC torsion
170.68	0.0212	0.0202	ν_{47}(a)	CCC bending + CC torsion
76.61	0.0095	0.0091	ν_{48}(a)	CCC bending + CC torsion

* energy with scaling factor correction (0.954) for CAMB3LYP [3].

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