Electronic Supplementary Material (ESI) for RSC Advances.

Fragment based electronic structural analysis of L-phenylalanine using calculated ionization spectroscopy and dual space analysis

Supplementary information

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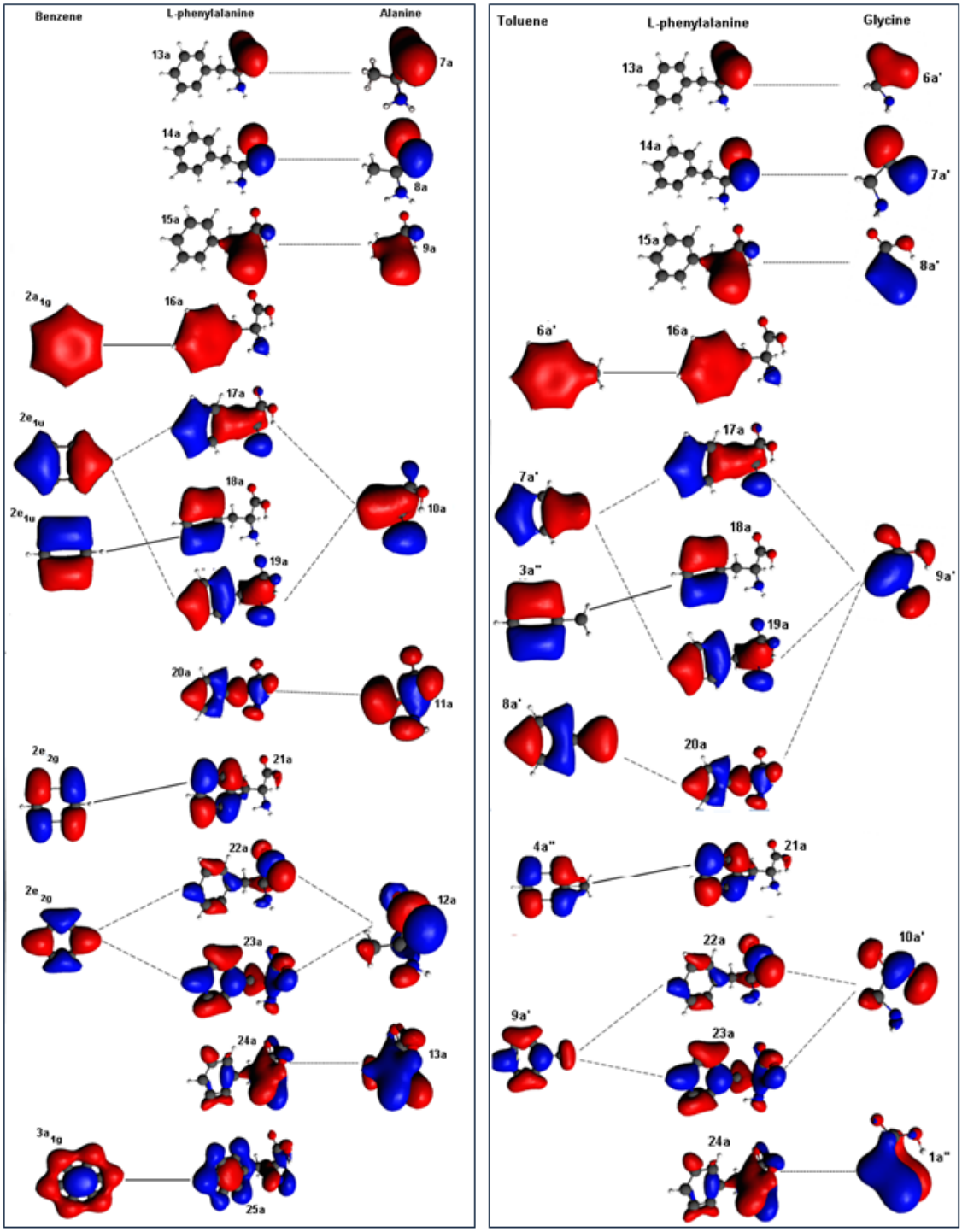
SI. 1: Selected geometric parameters of L-Phe and its fragments optimized using B3LYP/TZVP model along with the available experimental data.

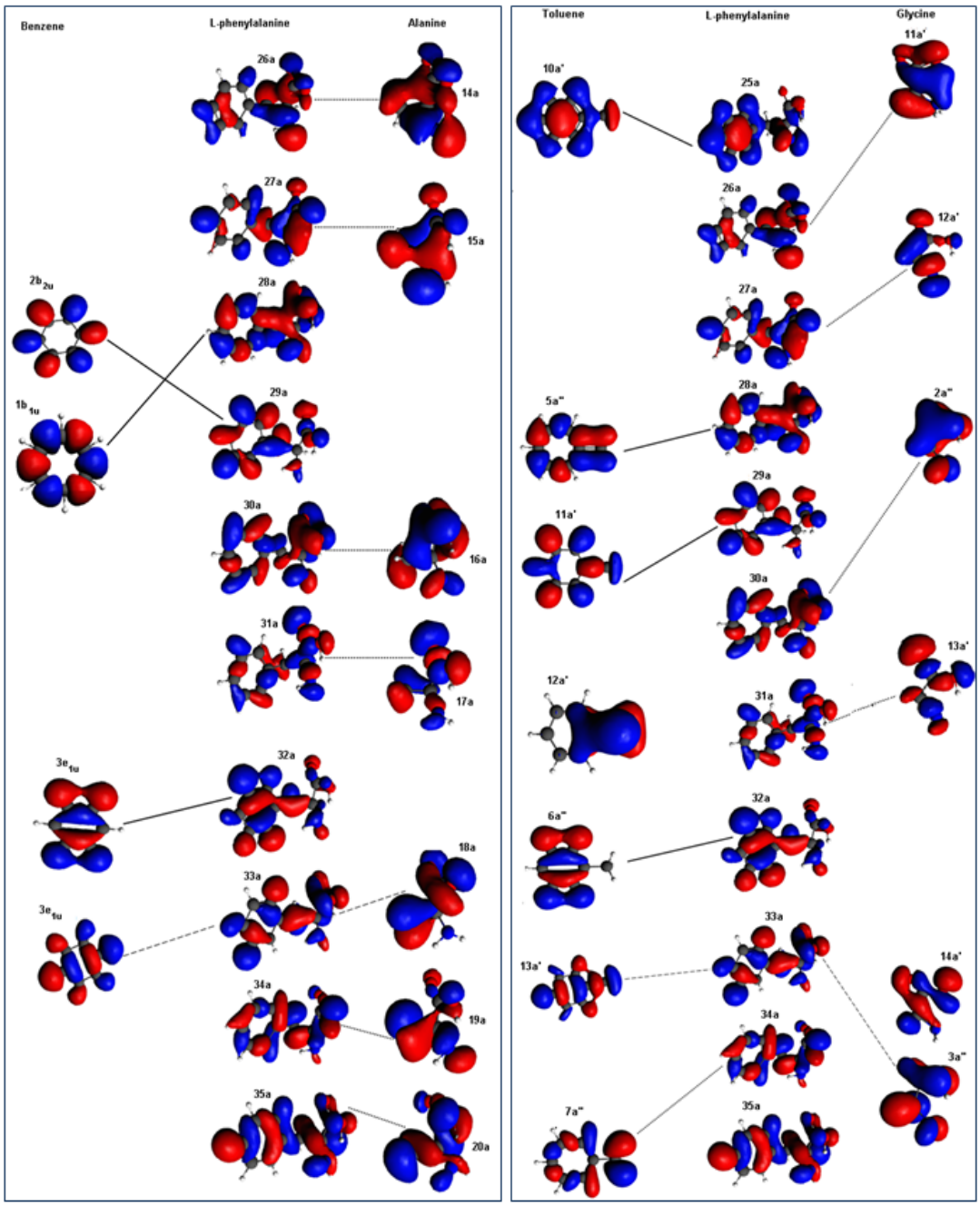
Parameters	L-Phe	Alanine		Glycine		
	This Work[a]	This Work[a]	Exp[b]	This Work[a]	Exp[b]	Other
$C_{(1)}$-$C_{(\alpha)}$ (Å)	1.55	1.54	1.51[c]	1.54	1.529[e]	1.52[g]
$C_{(\alpha)}$-$C_{(\beta)}$ (Å)	1.55	1.53	1.54[c]			
$C_{(\alpha)}$-N (Å)	1.47	1.46	1.47[c]	1.47	1.466[e]	1.45[g]
∠$C_{(1)}$-$C_{(\alpha)}$-$C_{(\beta)}$ /º	111.90	109.10				
∠$C_{(1)}$-$C_{(\alpha)}$-N /º	109.30	109.50	110.00[c]	111.60	113[e]	115.60[g]
∠O-$C_{(1)}$-$C_{(\alpha)}$-$H_{(1)}$/º	-102.00	-134.20		567.00		
∠O-$C_{(1)}$-$C_{(\alpha)}$-$C_{(\beta)}$ /º	40.00	108.70		-123.00		
	Phenyl	**Benzene**		**Toluene**		
$C_{(\gamma)}$-$C_{(2)}$ (Å)	1.40	1.39	1.39[d]	1.40		1.40[h]
$C_{(2)}$-$C_{(3)}$ (Å)	1.39			1.39		1.39[h]
$C_{(3)}$-$C_{(4)}$ (Å)	1.39			1.39		1.39[h]
$C_{(4)}$-$C_{(5)}$ (Å)	1.39			1.39	1.39[f]	1.39[h]
$C_{(5)}$-$C_{(6)}$ (Å)	1.39			1.39	1.39[f]	1.398[h]
$C_{(6)}$-$C_{(\gamma)}$ (Å)	1.40			1.40	1.39[f]	1.40[h]
R_6 (Å)	8.37	8.36	8.35[d]	8.36		8.35[h]
∠$C_{(\gamma)}$-$C_{(2)}$-$C_{(3)}$ /º	120.70	120.00		121.00		
∠$C_{(2)}$-$C_{(3)}$-$C_{(4)}$ /º	120.40			121.00		
∠$C_{(3)}$-$C_{(4)}$-$C_{(5)}$ /º	119.60			119.40	119.40[f]	
∠$C_{(4)}$-$C_{(5)}$-$C_{(6)}$ /º	120.00			121.00	120.20[f]	
∠$C_{(5)}$-$C_{(6)}$-$C_{(\gamma)}$ /º	121.10			121.00	120.60[f]	
∠$C_{(6)}$-$C_{(\gamma)}$-$C_{(2)}$ /º	118.30			118.60	119.00[f]	
∠$C_{(\gamma)}$-$C_{(2)}$-$C_{(3)}$-$C_{(4)}$ /º	-0.08	0.00		-0.11		
∠$C_{(2)}$-$C_{(3)}$-$C_{(4)}$-$C_{(5)}$ /º	-0.23			-0.08		
∠$C_{(3)}$-$C_{(4)}$-$C_{(5)}$-$C_{(6)}$ /º	0.23			0.08		
∠$C_{(4)}$-$C_{(5)}$-$C_{(6)}$-$C_{(\gamma)}$ º	-0.07			0.11		
∠$C_{(5)}$-$C_{(6)}$-$C_{(\gamma)}$-$C_{(2)}$ /º	-0.37			-0.28		

[a] B3LYP/TZVP model[1].
[b]Experimental structure may not be the same conformer investigated in this study. Therefore used only as a guide. See Ref. 2[2].
[c] Ref. 3[3] .
[d]MW spectrum[4].
[e]Ref. 5[5].
[f]Microwave spectrum[6].
[g]MP2 calculations[7].
[h]Ref. 8[8].

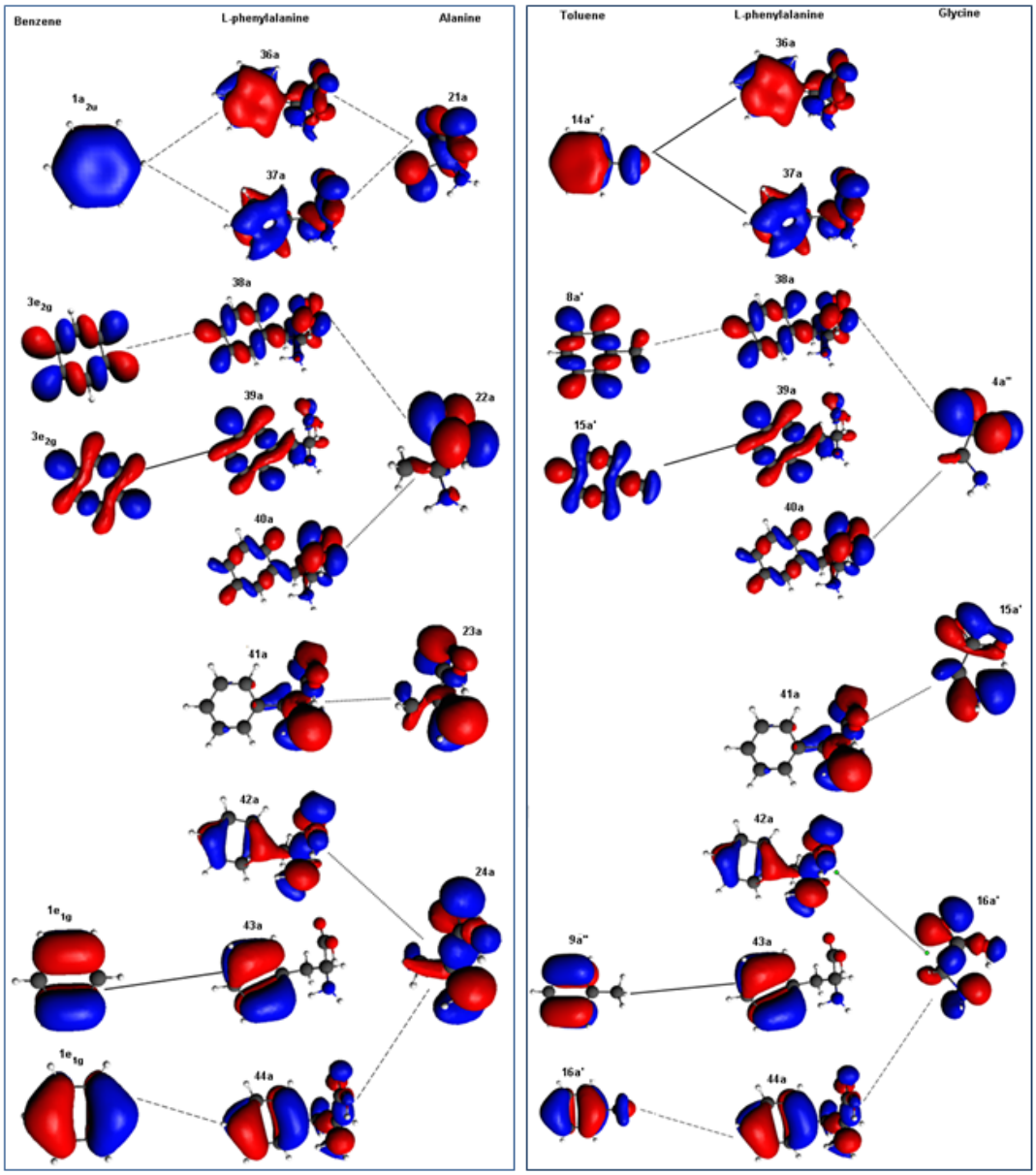
SI. 2: Valence orbital diagrams of L-Phe correlated with its fragment pairs: benzene/alanine and toluene/glycine. Note that the figures are presented on a mock energy scale.



SI. 2: Continued…



SI. 2: Continued…



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