Electronic supplementary information – 1 for

Dipole moment enhanced π–π stacking in fluorophenylacetylenes is carried over from gas-phase dimers to crystal structures propagated through liquid like clusters

Sumitra Singh,[a] Po-Jen Hsu,[b] Jer-Lai Kuo,*[b] and G. Naresh Patwari*[a]

[a] Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076 India.
E-mail: naresh@chem.iitb.ac.in

[b] Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.
E-mail: jlkuo@pub.iams.sinica.edu.tw

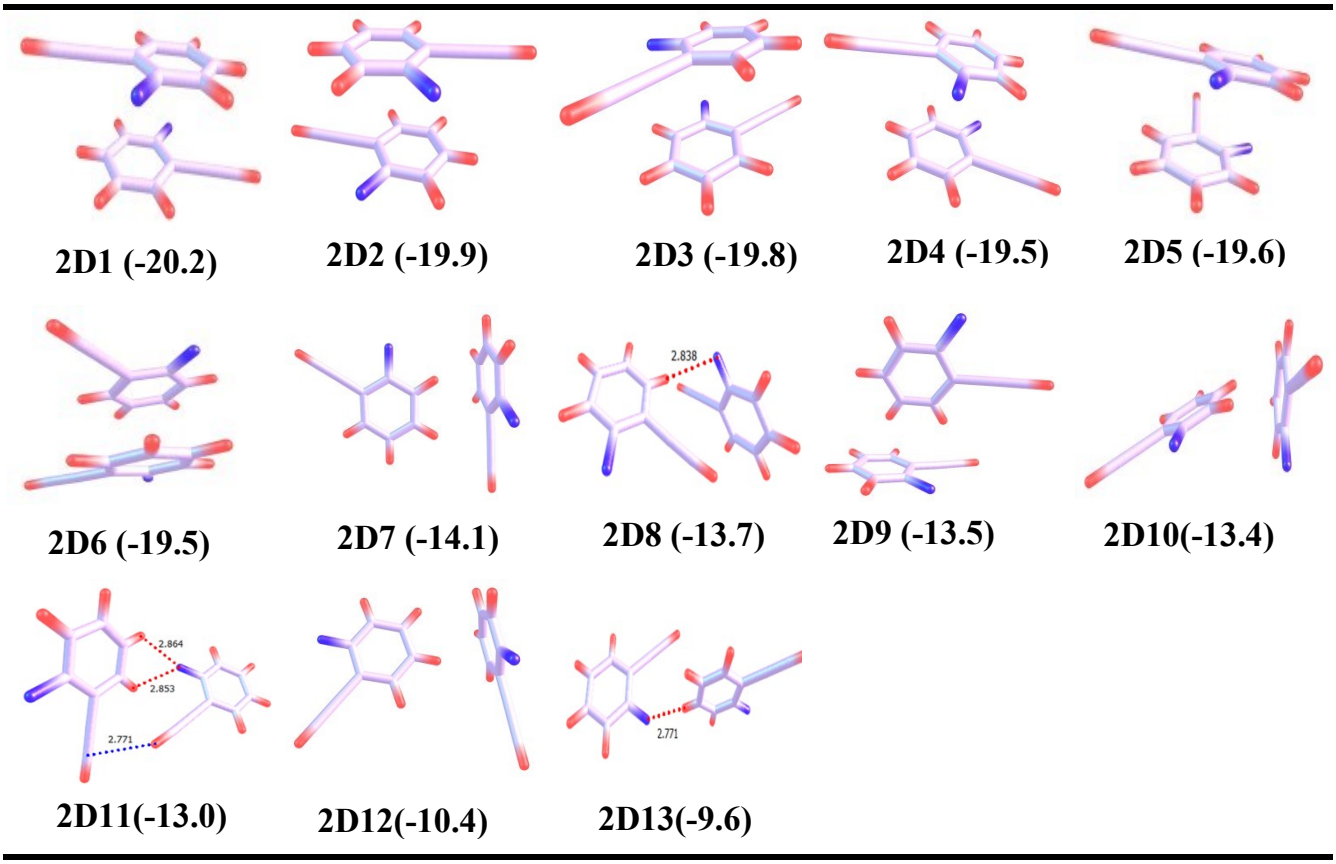

Fig. S1 Selected structures of 2-Fluorophenylacetylene dimers optimized at B97-D/aug-cc-pVDZ level of theory, for each structure the number in parenthesis is the ZPE and BSSE corrected stabilization energy in kJ mol^{-1}. Interaction with involvement of {Ac} CH and {Ar} CH groups are shown with blue and red dotted lines respectively with distance in Å.

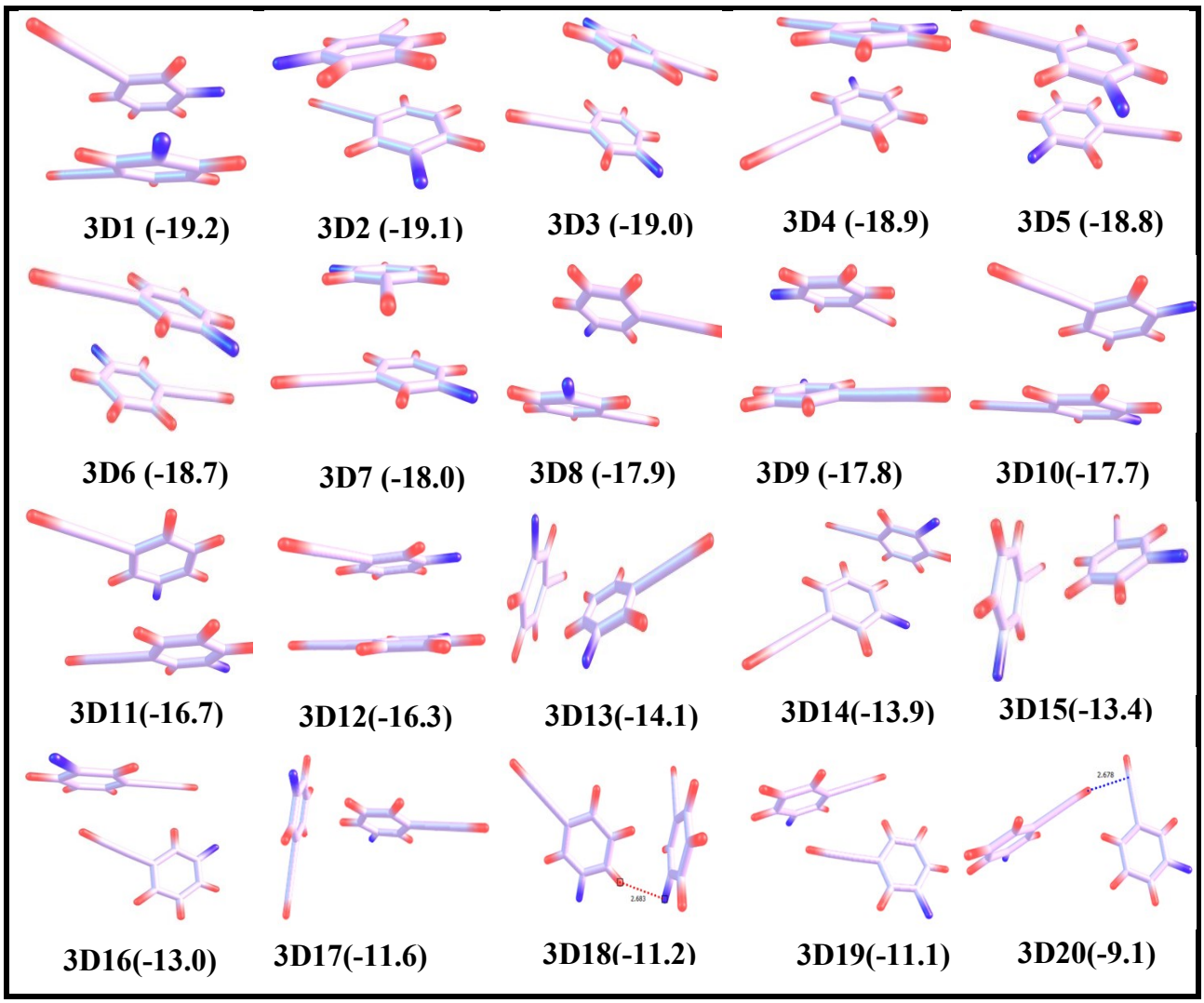

Fig. S2 Selected structures of 3-Fluorophenylacetylene dimers optimized at B97-D/aug-cc-pVDZ level of theory, for each structure the number in parenthesis is the ZPE and BSSE corrected stabilization energy in kJ mol^{-1}. Interaction with involvement of {Ac} CH and {Ar} CH groups are shown with blue and red dotted lines respectively with distance in Å.

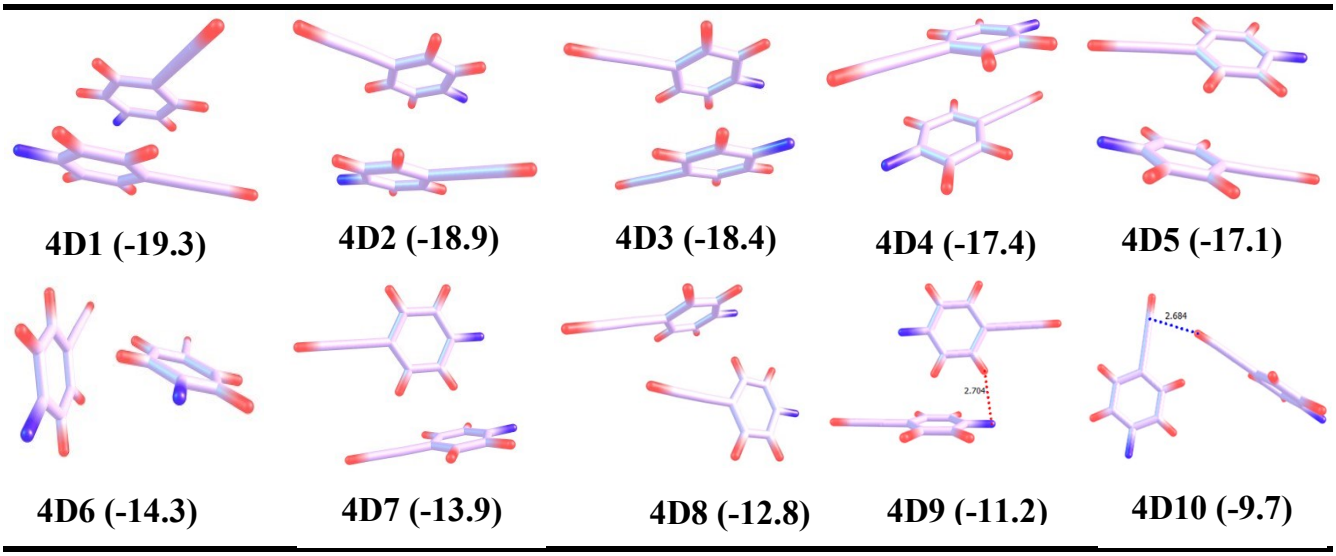

Fig. S3 Selected structures of 4-Fluorophenylacetylene dimers optimized at B97-D/aug-cc-pVDZ level of theory, for each structure the number in parenthesis is the ZPE and BSSE corrected stabilization energy in kJ mol^{-1}. Interaction with involvement of {Ac} CH and {Ar} CH groups are shown with blue and red dotted lines respectively with distance in Å.

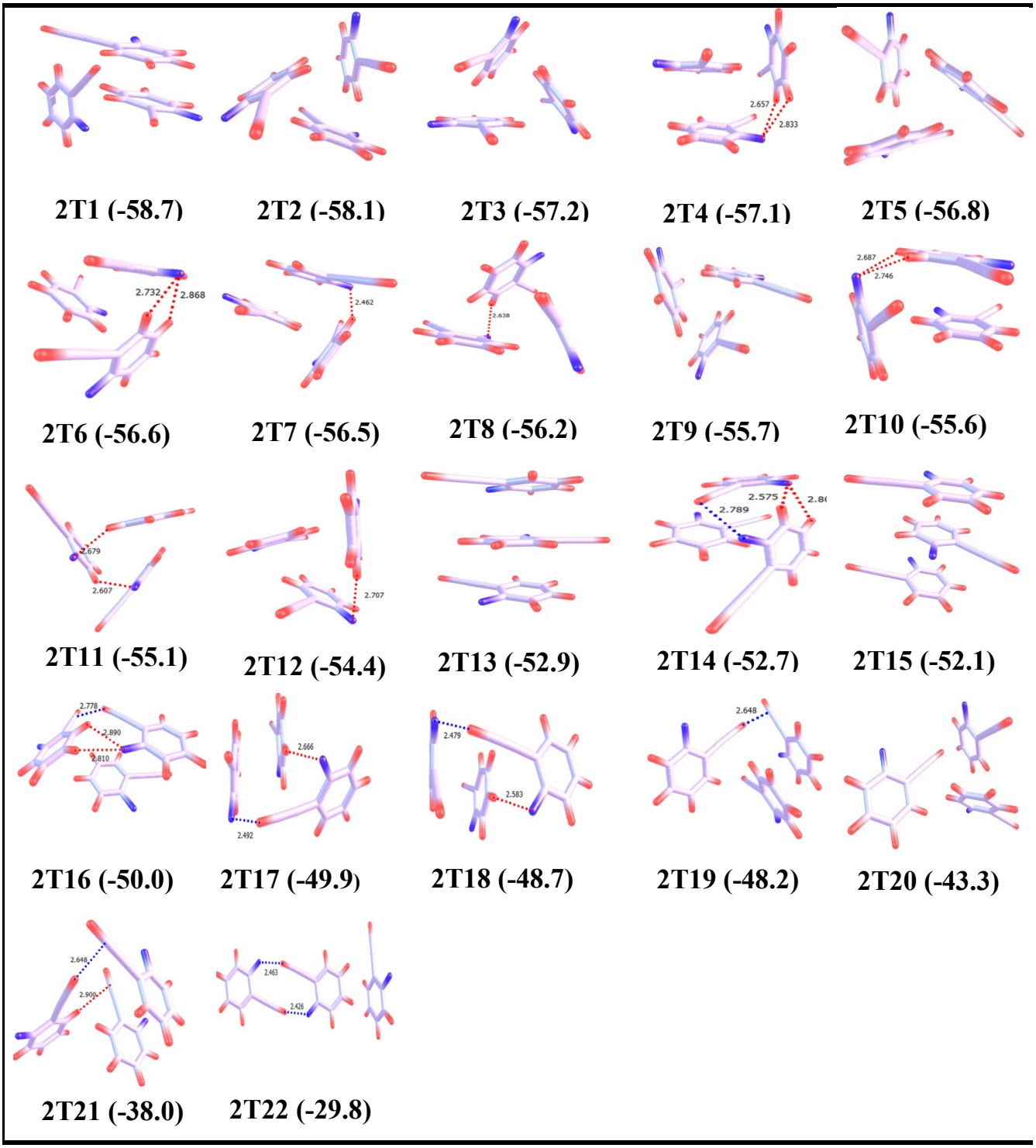

Fig. S4 Selected structures of 2-Fluorophenylacetylene trimers optimized at B97-D/aug-cc-pVDZ level of theory, for each structure the number in parenthesis is the ZPE and BSSE corrected stabilization energy in kJ mol^{-1}. Interaction with involvement of {Ac} CH and {Ar} CH groups are shown with blue and red dotted lines respectively with distance in Å.

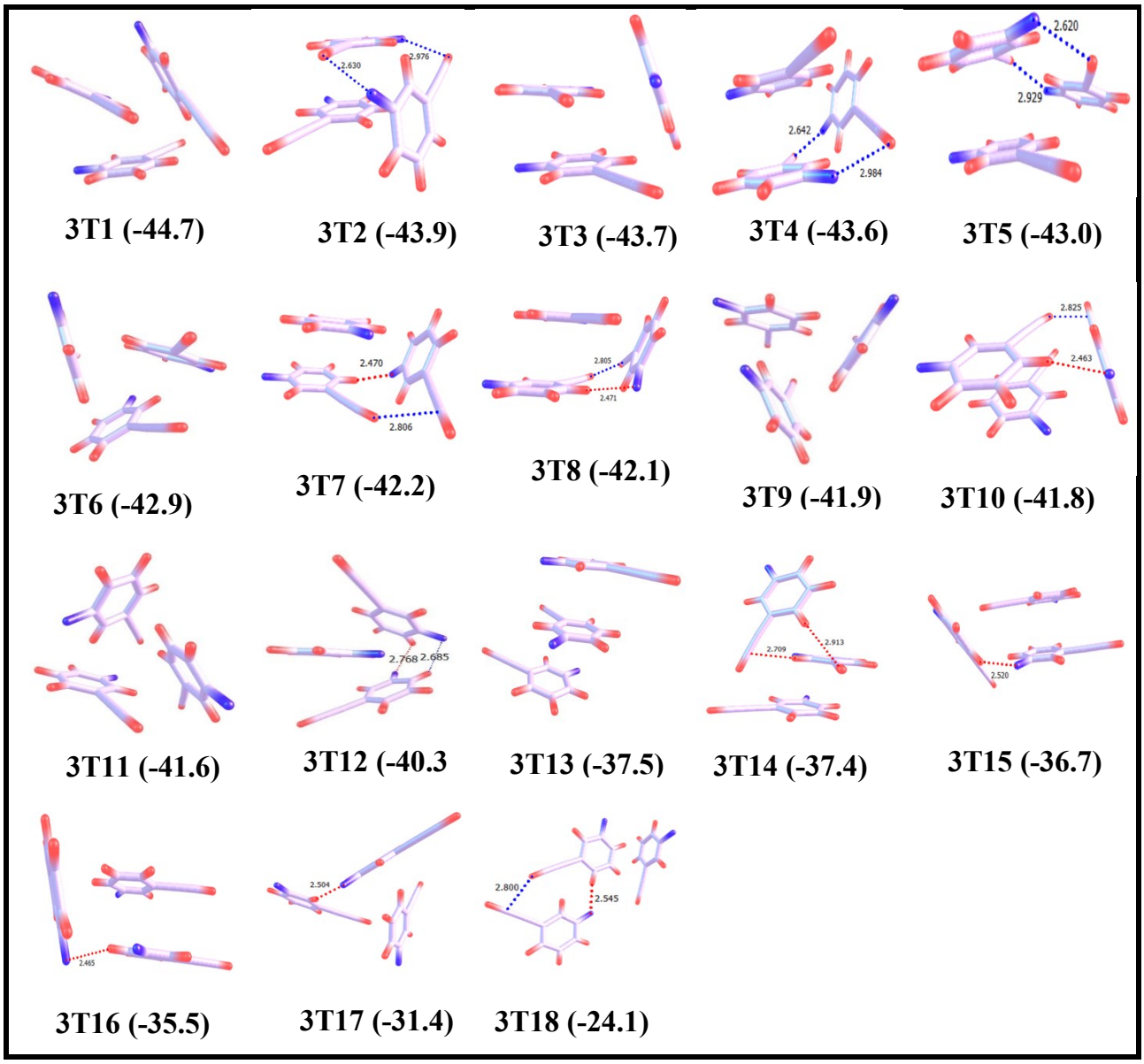

Fig. S5 Selected structures of 3-Fluorophenylacetylene trimers optimized at B97-D/aug-cc-pVDZ level of theory, for each structure the number in parenthesis is the ZPE and BSSE corrected stabilization energy in kJ mol^{-1}. Interaction with involvement of {Ac} CH and {Ar} CH groups are shown with blue and red dotted lines respectively with distance in Å.

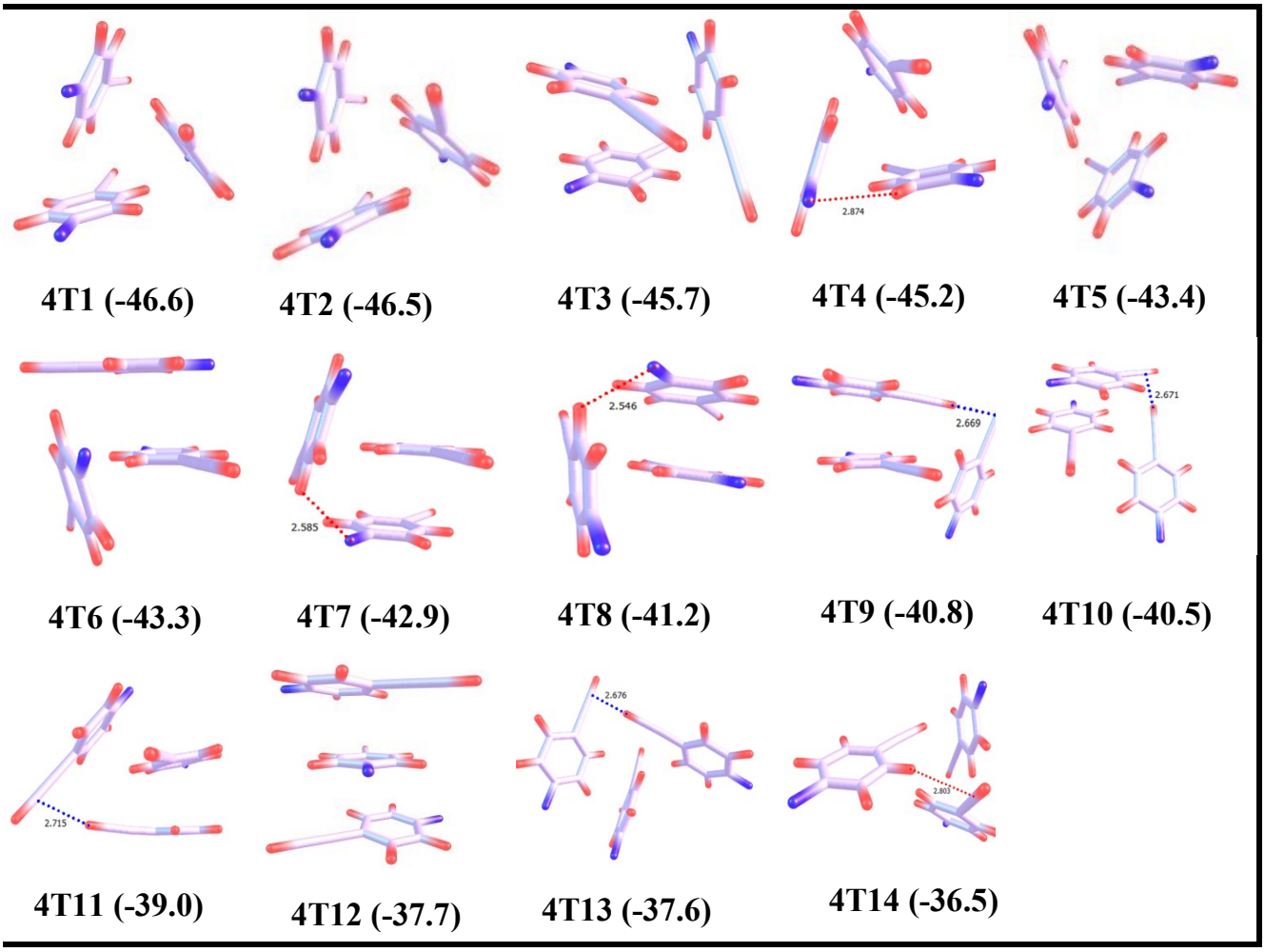

Fig. S6 Selected structures of 4-Fluorophenylacetylene trimers optimized at B97-D/aug-cc-pVDZ level of theory, for each structure the number in parenthesis is the ZPE and BSSE corrected stabilization energy in kJ mol^{-1}. Interaction with involvement of {Ac} CH and {Ar} CH groups are shown with blue and red dotted lines respectively with distance in Å.

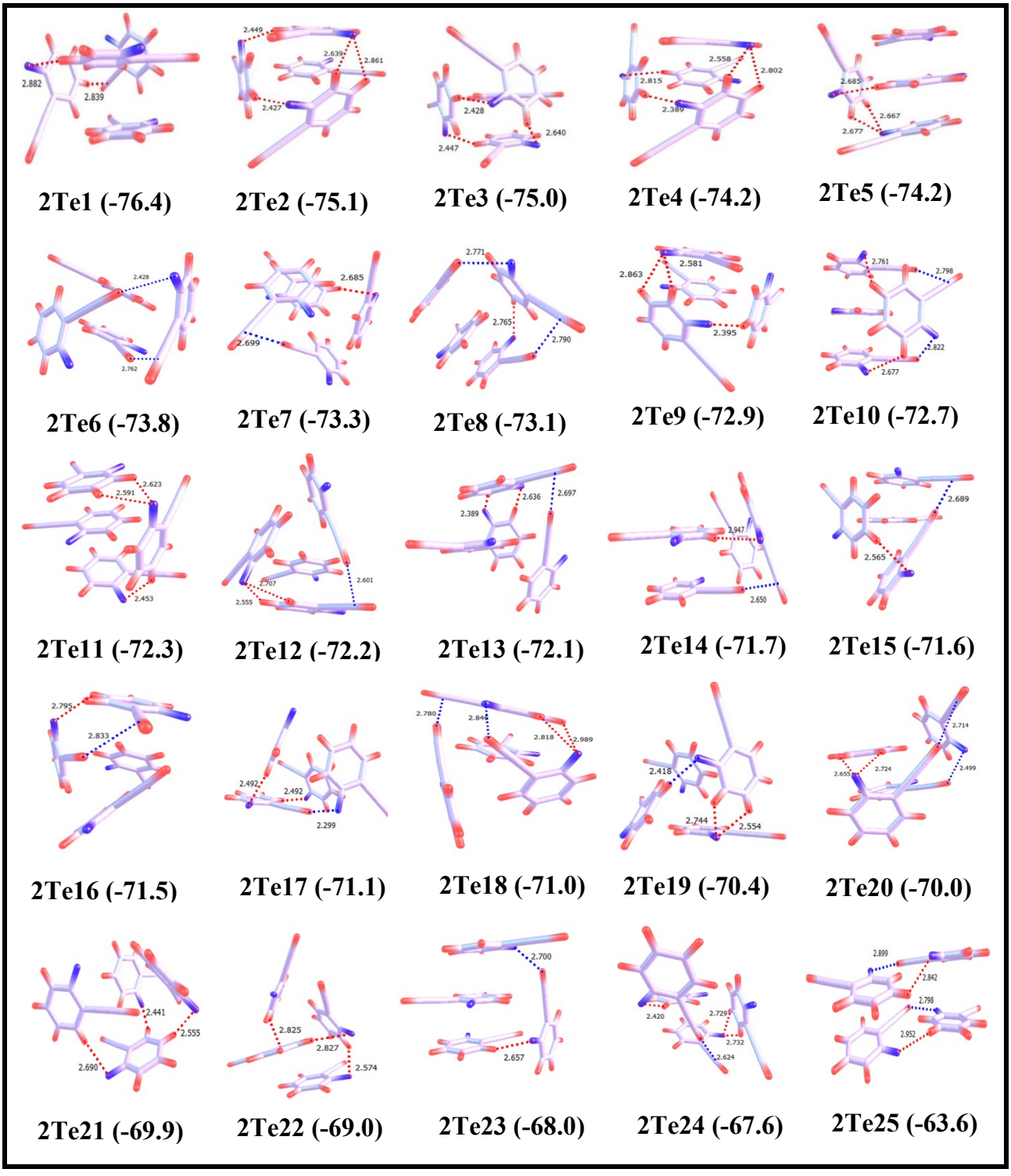

Fig. S7 Selected structures of 2-Fluorophenylacetylene tetramers optimized at B97-D/aug-cc-pVDZ level of theory, for each structure the number in parenthesis is the ZPE and BSSE corrected stabilization energy in kJ mol^{-1}. Interaction with involvement of {Ac} CH and {Ar} CH groups are shown with blue and red dotted lines respectively with distance in Å.

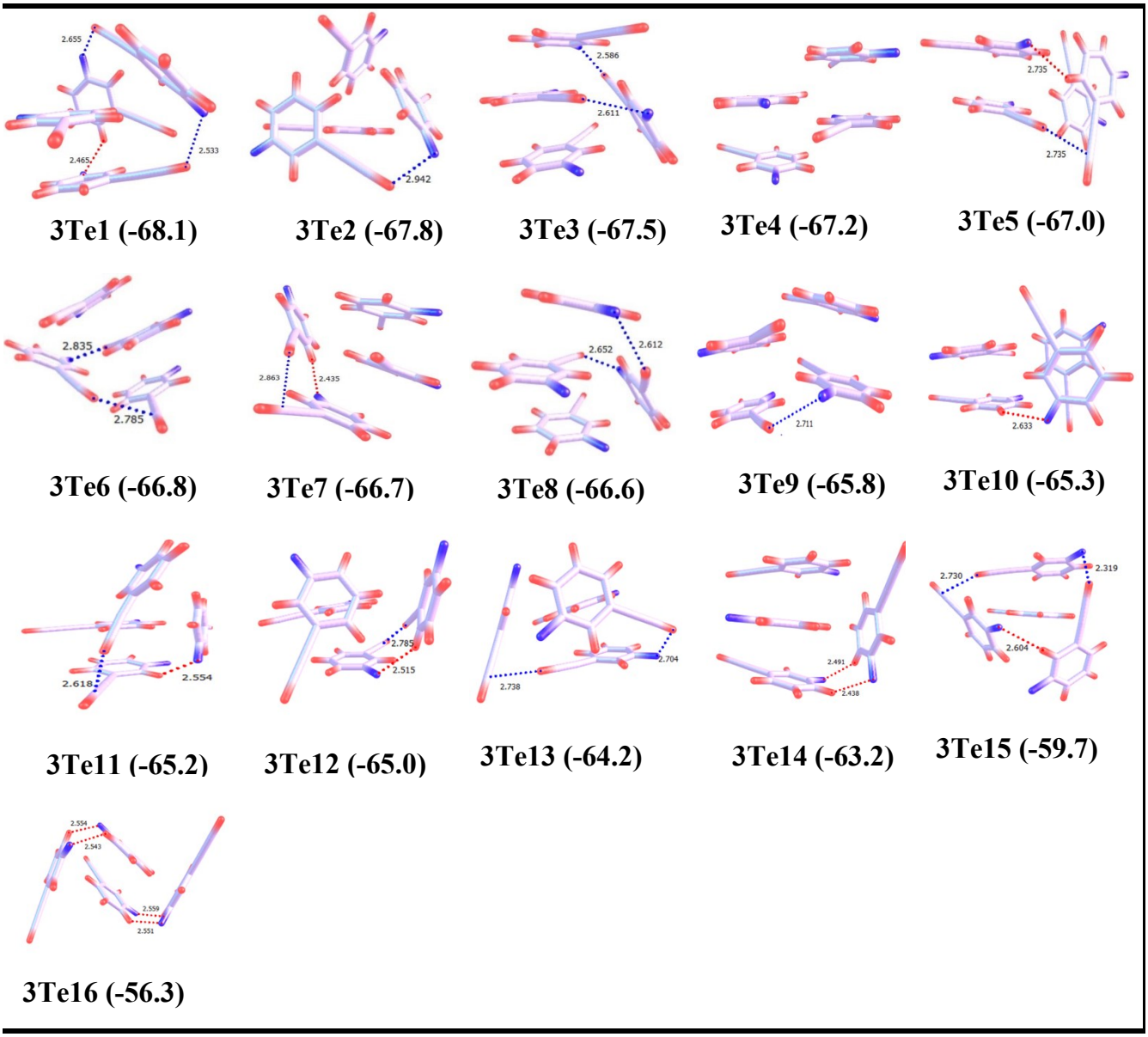

Fig. S8 Selected structures of 3-Fluorophenylacetylene tetramers optimized at B97-D/aug-cc-pVDZ level of theory, for each structure the number in parenthesis is the ZPE and BSSE corrected stabilization energy in kJ mol^{-1}. Interaction with involvement of {Ac} CH and {Ar} CH groups are shown with blue and red dotted lines respectively with distance in Å. Structures falling within 2kJ/mol energy range with respect to most stable structure with involvement of {Ac} CH groups to the interactions are highlighted.

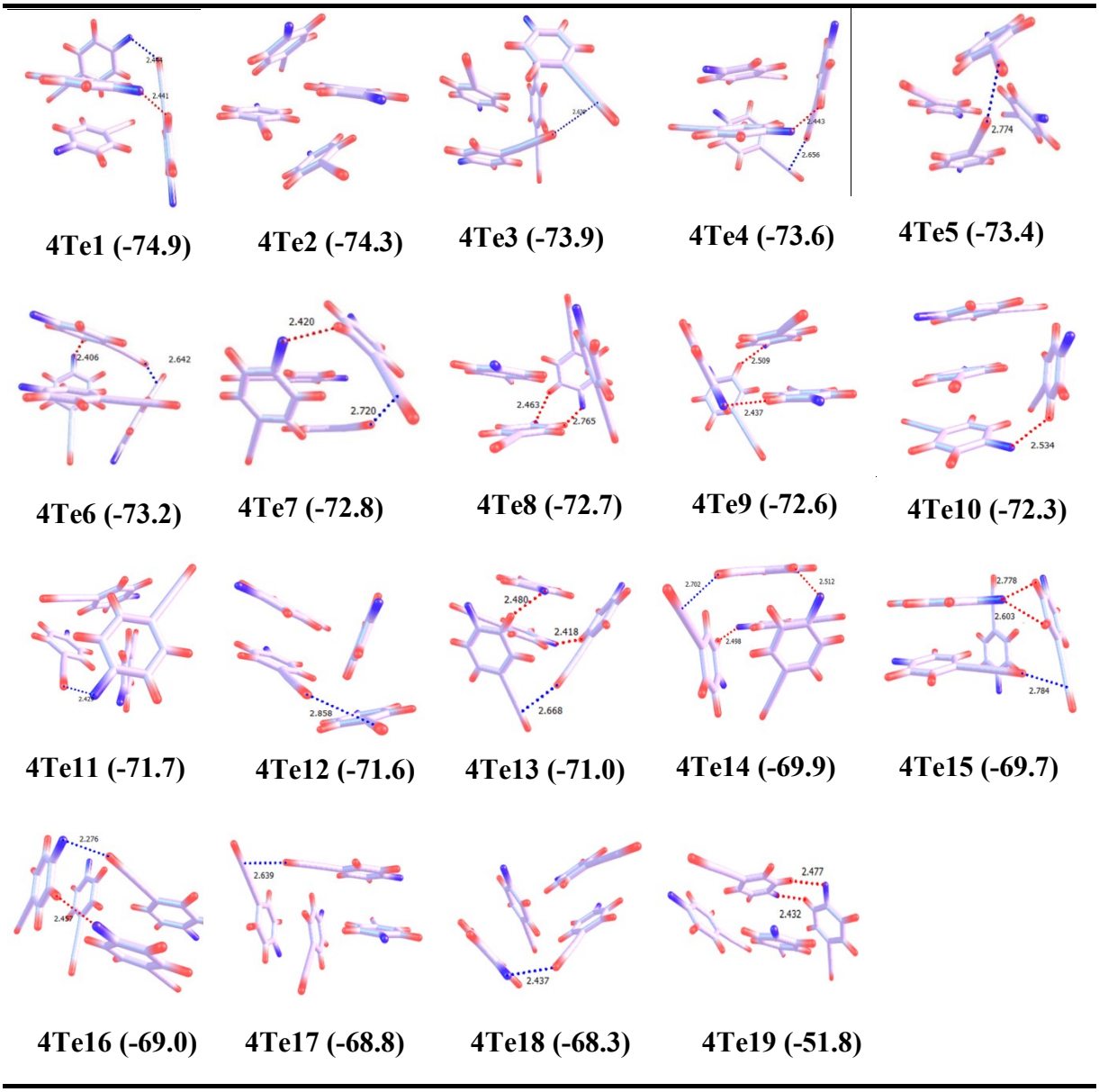

Fig. S9 Selected structures of 4-Fluorophenylacetylene tetramers optimized at B97-D/aug-cc-pVDZ level of theory, for each structure the number in parenthesis is the ZPE and BSSE corrected stabilization energy in kJ mol^{-1}. Interaction with involvement of {Ac} CH and {Ar} CH groups are shown with blue and red dotted lines respectively with distance in Å. Structures falling within 2 kJ/mol energy range with respect to most stable structure with involvement of {Ac} CH groups to the interactions are highlighted.