

Supplementary Material for „Shock Wave Study and Theoretical Modeling of the Thermal Decomposition of c-C₄F₈“

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Cartesian coordinates computed at the B3LYP/6-31G(2df) level

c-C₄F₈:

C:0.0003370693,-0.001003433,-0.0000057692
C:0.0000306353,0.0010438642,1.5714605562
C:1.5713994859,-0.0009789611,1.5538338775
C:1.5366435206,0.3290972813,0.0178084754
F:-0.7809774514,0.9031704939,-0.5817309238
F:-0.240596394,-1.2192885398,-0.4957252879
F:2.3028307529,-0.4318893606,-0.7569346175
F:1.769671572,1.6245823447,-0.2176068209
F:2.0695438407,-1.2193050376,1.7895064729
F:2.1617732405,0.9032180747,2.3285954562
F:-0.5752403091,-1.0463354839,2.1532152247
F:-0.4902142848,1.1421739543,2.0669363297

TS1:

C:0.,0.,0.
C:0.000000,0.000000,1.458420
C:1.506131,0.000000,2.016434
C:2.187786,1.257909,1.729536
F:2.864780,1.461889,0.636937
F:1.945439,2.333004,2.419514
F:1.361004,-0.173143,3.345227
F:2.172575,-1.038951,1.480046
F:-0.536496,1.131855,2.030796
F:-0.753077,-1.008854,1.968008
F:-0.941429,-0.662401,-0.630866
F:1.117367,0.041766,-0.695063

TS2:

C:0.,0.,0.
C:,0.000000,0.000000,1.443073
C:1.389432,0.000000,1.961812
C:2.151949,1.149087,1.30217:
F:3.271229,1.009459,0.70666:
F:1.844925,2.350965,1.58386:
F:1.434724,0.222247,3.292957
F:2.067362,-1.118827,1.645871
F:1.138417,1.077685,-0.436371
F:-0.659893,1.115561,1.912564
F:-1.059683,0.458977,-0.601455
F:0.463047,-1.070422,-0.599434

CF₂CF₂CF₂CF₂ (Singlet):

C:0.,0.,0.

C:0.,0.,1.32363795

C:3.6303314377,0.,0.5269007818

C:3.4724485763,-1.1658241209,1.133465446

F:2.6948397644,-2.1184824442,0.6723886513

F:4.0749826247,-1.4806705105,2.2568428759

F:3.02071862,0.3155764104,-0.5971777577

F:4.4056690554,0.9570963848,0.9841180823

F:-0.5167726642,0.9655752583,2.0494962535

F:0.5225141076,-0.970809692,2.0441301404

F:-0.515619383,0.9692562643,-0.7202780852

F:0.5193075467,-0.9675107907,-0.720507333

CF₂CF₂CF₂CF₂ (Triplet):

C:0.,0.,0.

C:0.,0.,1.51796502

C:1.4271321286,0.,2.1179031544

C:1.4387869127,0.2885488516,3.6081451462

F:2.6505505635,0.4116820106,4.1113240222

F:0.674506632,-0.5001022476,4.3379247903

F:2.0034616477,-1.1989616634,1.855059251

F:2.152843147,0.9552610977,1.5040407504

F:-0.642321595,1.1094111215,1.9334601858

F:-0.6682595599,-1.0771780166,1.9994927764

F:-1.2018747006,0.1216805095,-0.5267000406

F:0.6931815661,-0.9715059122,-0.5606681829