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Supplemental data for

Accurate heats of formation for SF_n, SF_n⁺, and SF_n⁻ for n=1-6
 Charles W. Bauschlicher, Jr. and Alessandra Ricca

SF_n, SF_n⁺, and SF_n⁻, n=1-6 gasphase thermochemistry data

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*****
*   The data is fit using the Chemkin fitting program and following their
*   constrained three step procedure. There are seven coefficients for each
*   temperature range. See R. J. Kee, F. M. Rupley, and J. A. Miller, Sandia
*   National Laboratories, SAND87-8215B (1991)
*
*   The first card contains tile, number of atoms of each type, low and high
*   temperature used in the fit and the change over temperature for the lower
*   and upper ranges. This is followed the the 7 coefficient for the upper
*   range and the 7 coefficients for the lower range.
*   coefficients (a1-a7) are defined as
*
*   Cp/R=a1+a2*T+a3*T**2+a4*T**3+a5*T**4
*   H^0/(RT)= a1+(a2*T)/2+(a3*T**2)/3+(a4*T**3)/5+(a5*T**4)/5+a6/T
*   S^0/R=a1*ln(T)+a2*T+(a3*T**2)/2+(a4*T**3)/3+(a5*T**4)/4+a7
*
*****
SF6          OS   1F   6   0   OG   300.000  4000.000 1000.00   0 1
  0.15275723E+02 0.46833914E-02-0.23555025E-05 0.53452599E-09-0.45320365E-13   2
-0.15221983E+06-0.54088009E+02-0.24939622E+01 0.80279379E-01-0.12936295E-03   3
  0.98840191E-07-0.29169844E-10-0.14866384E+06 0.31080936E+02   4
SF5          OS   1F   5   0   OG   300.000  4000.000 1000.00   0 1
  0.13636069E+02 0.29702499E-02-0.14917127E-05 0.33800363E-09-0.28618266E-13   2
-0.10648093E+06-0.41577729E+02 0.54189973E+00 0.59906811E-01-0.98835059E-04   3
  0.76591688E-07-0.22781349E-10-0.10392014E+06 0.20878987E+02   4
SF4          OS   1F   4   0   OG   300.000  4000.000 1000.00   0 1
  0.11055023E+02 0.24466158E-02-0.12302283E-05 0.27906867E-09-0.23651832E-13   2
-0.96186308E+05-0.28531463E+02 0.10847671E+01 0.45276377E-01-0.73737838E-04   3
  0.56686027E-07-0.16782506E-10-0.94211698E+05 0.19152061E+02   4
SF3          OS   1F   3   0   OG   300.000  4000.000 1000.00   0 1
  0.88438951E+01 0.14543225E-02-0.73103144E-06 0.16576828E-09-0.14044353E-13   2
-0.56038539E+05-0.15330225E+02 0.26484025E+01 0.28231026E-01-0.46278998E-04   3
  0.35713561E-07-0.10595081E-10-0.54819484E+05 0.14259997E+02   4
SF2          OS   1F   2   0   OG   300.000  4000.000 1000.00   0 1
  0.61106365E+01 0.11227659E-02-0.56653056E-06 0.12891926E-09-0.10956290E-13   2
-0.37522127E+05-0.42999136E+01 0.24912109E+01 0.15986234E-01-0.24772398E-04   3
  0.18427952E-07-0.53481645E-11-0.36773129E+05 0.13176283E+02   4
SF          OS   1F   1   0   OG   300.000  4000.000 1000.00   0 1
  0.43880420E+01 0.13951450E-03-0.69289214E-07 0.15543556E-10-0.13046048E-14   2
-0.97902522E+03 0.20216979E+01 0.34427989E+01 0.44797267E-02-0.78114671E-05   3
  0.62602350E-08-0.18987873E-11-0.80483860E+03 0.64748895E+01   4
SF6+         OS   1F   6   0   OG   300.000  3900.000 1000.00   0 1
  0.15378154E+02 0.46191483E-02-0.23636275E-05 0.54681916E-09-0.47330758E-13   2
  0.13206923E+05-0.43348909E+02 0.22274939E+01 0.58302428E-01-0.89388478E-04   3
  0.66149322E-07-0.19157602E-10 0.15945655E+05 0.20231844E+02   4
SF5+         OS   1F   5   0   OG   300.000  4000.000 1000.00   0 1
  0.12443206E+02 0.44730451E-02-0.22522815E-05 0.51183435E-09-0.43458635E-13   2
  0.52384473E+04-0.37049495E+02-0.67026530E+00 0.57846470E-01-0.88683863E-04   3
  0.65708607E-07-0.19068603E-10 0.79815688E+04 0.26401548E+02   4
SF4+         OS   1F   4   0   OG   300.000  4000.000 1000.00   0 1
  0.10852701E+02 0.26997913E-02-0.13581384E-05 0.30831449E-09-0.26151761E-13   2
  0.43112916E+05-0.26736441E+02 0.15320111E+01 0.41811016E-01-0.66359717E-04   3
  0.50260559E-07-0.14767352E-10 0.45005366E+05 0.18072723E+02   4
SF3+         OS   1F   3   0   OG   300.000  4000.000 1000.00   0 1
  0.80105196E+01 0.25047119E-02-0.12625719E-05 0.28721343E-09-0.24408408E-13   2
  0.40646531E+05-0.14278134E+02 0.14966844E+01 0.28274932E-01-0.41935632E-04   3
  0.30378016E-07-0.86985348E-11 0.42045068E+05 0.17422420E+02   4
SF2+         OS   1F   2   0   OG   300.000  4000.000 1000.00   0 1
  0.57637543E+01 0.15576409E-02-0.78604090E-06 0.17901450E-09-0.15229335E-13   2
  0.81452200E+05-0.21754564E+01 0.24613589E+01 0.13898179E-01-0.19202924E-04   3

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0.13200747E-07-0.36582220E-11	0.82196453E+05	0.14074757E+02	4	
SF+ OS 1F 1 0 OG	300.000	4000.000	1000.00	0 1
0.38893766E+01	0.76963163E-03-0.38872952E-06	0.88625057E-10-0.75475521E-14	2	
0.11882213E+06	0.44433954E+01	0.27414653E+01	0.45032385E-02-0.51053158E-05	3
0.29126224E-08-0.70065413E-12	0.11910806E+06	0.10229517E+02	4	
SF6- OS 1F 6 0 OG	300.000	4000.000	1000.00	0 1
0.17371987E+02	0.20377977E-02-0.10188255E-05	0.22989366E-09-0.19393175E-13	2	
-0.16319499E+06-0.57263332E+02	0.59826559E+01	0.53125417E-01-0.90515569E-04	3	
0.71517847E-07-0.21508892E-10-0.16104131E+06-0.33181409E+01			4	
SF5- OS 1F 5 0 OG	300.000	4000.000	1000.00	0 1
0.14352742E+02	0.20622321E-02-0.10314892E-05	0.23285007E-09-0.19650171E-13	2	
-0.15404590E+06-0.44194693E+02	0.31282174E+01	0.52268570E-01-0.88798608E-04	3	
0.70046175E-07-0.21047668E-10-0.15191656E+06	0.90046972E+01		4	
SF4- OS 1F 4 0 OG	300.000	4000.000	1000.00	0 1
0.12084101E+02	0.11428834E-02-0.56951822E-06	0.12812625E-09-0.10780139E-13	2	
-0.11299306E+06-0.30778209E+02	0.48632077E+01	0.33988941E-01-0.58728126E-04	3	
0.46790740E-07-0.14139951E-10-0.11164881E+06	0.33132884E+01		4	
SF3- OS 1F 3 0 OG	300.000	4000.000	1000.00	0 1
0.92349126E+01	0.95703468E-03-0.47817557E-06	0.10784198E-09-0.90933580E-14	2	
-0.92294215E+05-0.18226305E+02	0.38326359E+01	0.25238145E-01-0.43087218E-04	3	
0.34091703E-07-0.10262745E-10-0.91274714E+05	0.73501711E+01		4	
SF2- OS 1F 2 0 OG	300.000	4000.000	1000.00	0 1
0.72192693E+01	0.34860205E-03-0.17272397E-06	0.38661395E-10-0.32385435E-14	2	
-0.54172205E+05-0.96596539E+01	0.46547268E+01	0.12207188E-01-0.21434355E-04	3	
0.17244336E-07-0.52413257E-11-0.53703546E+05	0.24021048E+01		4	
SF- OS 1F 1 0 OG	300.000	4000.000	1000.00	0 1
0.42423865E+01	0.32479546E-03-0.16338595E-06	0.37065394E-10-0.31411016E-14	2	
-0.28319626E+05	0.19233029E+01	0.27874202E+01	0.66344980E-02-0.10916430E-04	3
0.84339110E-08-0.25016789E-11-0.28034666E+05	0.88663594E+01		4	