Supplementary Material (ESI) for *PCCP*

Supporting Information File

Modelling Doped (Ni, Pd, Pt) Sulfur-Nitrolic Systems as New Motifs for Storage of Hydrogen

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Available Information:

1. Ground State Optimized geometries (at various levels of theory) and Energies.
2. Harmonic Frequencies.
3. Complete Reference for reference 33.

S_2N_2

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	0.000000	1.180751
16	0.000000	0.000000	-1.180751
7	0.000000	1.179405	0.000000
7	0.000000	-1.179405	0.000000

E(B3LYP/6-31+g(d,p)) = -905.773838690 Hartree

Vibrational Frequencies (in cm^{-1}): 452.9734 625.7025 654.0806 755.6007 920.1363 922.3112

$S_3N_3^-$

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	1.689141	-0.067842
16	1.462839	-0.844570	-0.067842
16	-1.462839	-0.844570	-0.067842
7	1.430576	0.825950	0.155067
7	-1.430582	0.825940	0.155067
7	0.000000	-1.651891	0.155067

E(MP2/6-31+g(d,p)) = -1356.6998972 Hartree

Vibrational Frequencies (in cm^{-1}): 177.6025 177.6025 296.2314 360.5968 360.5968 529.1309 659.1083 700.5900 700.590

$S_3N_3^-$

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	0.000000	1.683293	-0.042850
16	1.457774	-0.841646	-0.042850
16	-1.457774	-0.841646	-0.042850
7	1.409315	0.813767	0.097944
7	-1.409315	0.813767	0.097944
7	0.000000	-1.627238	0.097944

E(B3LYP/6-31+g(d,p)) = -1358.76903562 Hartree

Vibrational Frequencies (in cm^{-1}): 110.1508 110.1508 165.7850 372.5873 372.5873 562.0153 606.5959 606.5959 692.5165

$S_3N_3^-$

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	1.430747	0.826042	0.000000
16	-1.430747	0.826042	0.000000
16	0.000000	-1.652085	0.000000
7	0.000000	1.556568	0.000000
7	1.348027	-0.778284	0.000000
7	-1.348027	-0.778284	0.000000

E(HF/6-31+g(d,p)) = -1355.73065637 Hartree

Vibrational Frequencies (in cm^{-1}): 145.6867 145.6867 185.5533 428.6610 428.6610 674.9271 674.9271 675.6317 807.5378

$S_4N_4^{2+}$

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	1.543220	1.543220	0.000000
16	-1.543220	-1.543220	0.000000
16	1.543220	-1.543220	0.000000
16	-1.543220	1.543220	0.000000
7	0.000000	1.909239	0.000000
7	1.909239	0.000000	0.000000
7	-1.909239	0.000000	0.000000
7	0.000000	-1.909239	0.000000

E(B3LYP/6-31+g(d,p)) = -1810.83753553 Hartree

Vibrational Frequencies (in cm^{-1}): 61.1476 128.3552 168.8538 221.2926 407.1237 425.1589 425.1589 426.1079 426.1079

$S_4N_4^{2-}$

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-1.423371	-0.117561	-1.622465
16	-1.578891	-0.034519	1.407518
16	1.578891	0.034519	-1.407518

16	1.423371	0.117561	1.622465
7	-1.688239	-0.811009	-0.127902
7	0.141559	0.073462	-2.245884
7	1.688239	0.811009	0.127902
7	-0.141559	-0.073462	2.245884

E(B3LYP/6-31+g(d,p)) = -1811.57282710 Hartree

Vibrational Frequencies (in cm^{-1}): 41.2831 53.4242 80.8793 163.8112 200.9082 262.7638 308.4387 384.2832 467.6903

S_2N_2 + $2H_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	1.188914	0.000000	0.000000
16	-1.188914	0.000000	0.000000
7	0.000000	0.000000	1.198400
7	0.000000	0.000000	-1.198400
1	0.000000	3.175114	-0.367611
1	0.000000	3.175114	0.367611
1	0.000000	-3.175114	-0.367611
1	0.000000	-3.175114	0.367611

E(MP2/6-31+g(d,p)) = -906.024629820 Hartree

Vibrational Frequencies (in cm^{-1}): 47.3040 61.8656 100.1580 116.6759 117.1555 120.8050 135.5860 137.0448 145.9603

$S_4N_4^{2+}$ +2H_2

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	1.54826200	1.54826200	0.00000000
16	-1.54826200	-1.54826200	0.00000000
16	1.54826200	-1.54826200	0.00000000
16	-1.54826200	1.54826200	0.00000000
7	0.00000000	1.94927800	0.00000000
7	1.94927800	0.00000000	0.00000000
7	-1.94927800	0.00000000	0.00000000
7	0.00000000	-1.94927800	0.00000000
1	0.00000000	0.00000000	2.34007400
1	0.00000000	0.00000000	3.07805500
1	0.00000000	0.00000000	-2.34007400
1	0.00000000	0.00000000	-3.07805500

E(MP2/6-31+g(d,p)) = -1810.43067804 Hartree

Vibrational Frequencies (in cm^{-1}): 54.2984 91.8927 91.8927 108.6794 108.6794 149.2113 159.5969 198.0359 205.2093

S_2N_2 +Ni+3H_2

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-0.017780	1.360407	1.197581

16	-0.017780	1.360407	-1.197581
7	0.050567	0.193581	0.000000
7	-0.070941	2.515160	0.000000
1	-0.121297	-1.874368	1.494758
1	-0.121297	-1.874368	-1.494758
1	1.615136	-2.030417	-0.399132
28	-0.017780	-1.770235	0.000000
1	1.615136	-2.030417	0.399132
1	-1.411325	-1.976463	0.000000
1	-0.366911	-3.141595	0.000000

E(B3LYP/split-basis) = -1078.81465353 Hartree

Vibrational Frequencies (in cm^{-1}): 59.8253 96.7696 112.5746 229.9559 287.2986 362.8311 392.4692 456.1530 468.5490

S_2N_2 +Pd+3H_2

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-0.019130	1.804735	1.196057
16	-0.019130	1.804735	-1.196057
7	0.071837	0.639460	0.000000
7	-0.095603	2.959486	0.000000
46	-0.019130	-1.554995	0.000000
1	-0.268347	-3.056248	0.000000
1	-0.135525	-1.647869	1.633505
1	-1.528839	-1.686635	0.000000
1	1.863361	-1.687889	-0.392965
1	-0.135525	-1.647869	-1.633505

1	1.863361	-1.687889	0.392965

E(B3LYP/split-basis) = -1036.66505059 Hartree

Vibrational Frequencies (in cm^{-1}): 34.8329 82.3223 91.2614 173.5262
294.5380 381.9204 433.9928 452.3756 483.6843

S_2N_2 +Pt+$3H_2$

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-2.207537	-1.195837	0.000000
16	-2.197943	1.196840	0.000000
7	-1.036724	-0.003927	-0.000255
7	-3.358987	0.005149	0.000000
1	1.263809	-1.310926	-0.951968
1	1.248725	1.621516	-0.008055
1	1.249834	0.499030	1.540938
78	1.182854	-0.000326	0.000000
1	1.263433	-1.297838	0.969702
1	1.250238	0.481655	-1.546448
1	2.719025	0.007413	-0.000798

E(B3LYP/split-basis) = -1029.13755645 Hartree

Vibrational Frequencies (in cm^{-1}): 8.1783 99.9645 102.8116 161.7897
400.8790 411.3685 450.1117 471.1522 512.2589

Complete Reference 33:

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Gaussian 03, Revision C.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.