Supporting Information Available:

(Total 5 pages)

Reactivity of [1,2-benzisotellurazol-3(2H)-one] with the Peroxynitrous Acid: Comparison with their Ebselen Analogues.

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Table 1S. The bond lengths (in Å) in the molecules M_2 and MO (where M= S, Se and Te) calculated at the B3LYP level with various basis sets.

Molecules	BS1[a)]	6-311+G(3df,p)	aug-cc-pvqz	Exp.[b)]
S_2	1.9273	1.9025	1.9072	1.887
Se_2	2.1995	2.1863		2.166
Te_2	2.6521			2.556
SO	1.5102	1.4882	1.4916	1.481
SeO	1.6621	1.6467		1.649
TeO	1.8643			1.825

a) BS1 = {SDD(Te) + $[6\text{-}311+G(d,p)]_{O,\,S,\,Se}$}, see text for more details.
b) See Ref. [27]

Table 2S. The M-M and M-O bond energies (in kcal/mol) of the M_2 and MO molecules (M = S, Se and Te), respectively, calculated at the B3LYP and CCSD(T) levels using various basis sets. In the CCSD(T) calculations the B3LYP optimized geometries were used.

Mol.	BS1[a)]			6-311+G(3df,p)			aug-cc-pvqz		
	B3LYP		CCSD(T)	B3LYP		CCSD(T)	B3LYP		CCSD(T)
	ΔE[b)]	ΔH[c)]	ΔE[b)]	ΔE[b)]	ΔH[c)]	ΔE[b)]	ΔE[b)]	ΔH[c)]	ΔE[b)]
S_2	94.1	93.9	80.7	103.1	102.9	95.4	102.2	102.0	99.2
				Experiment:[a)]		*101.65*			
Se_2	82.7	82.9	68.6	84.5	84.2	76.7			
				Experiment:[a)]		*92.94*			
Te_2	55.6	55.9	36.8						
				Experiment:[a)]		*62.1 ± 1.2*			
SO	115.2	114.5	102.9	126.5	125.7	119.1	125.4	124.6	121.5
				Experiment:[a)]		*124.7 ± 2.3*			
SeO	100.0	99.5	85.8	107.1	106.6	100.4			
				Experiment:[a)]		*111 ± 5.1*			
TeO	78.1	77.9	51.2						
				Experiment:[a)]		*89.9 ± 5.0*			

a) see footnotes for Table 1S.
b) These numbers do not include zero-point energy and temperature corrections.
c) These numbers include zero-point energy and temperature corrections.

Table 3S. The B3LYP/{[6-311+G(d,p)]$_{\text{For all atoms}}$ + SDD (Te)} calculated Cartesian coordinates (in Å) of all structures reported in the paper.

NO_2

N	0.00000	0.00000	0.32195
O	0.00000	1.09986	-0.14085
O	0.00000	-1.09986	-0.14085

***cis*-HOONO**

O	-1.31852	-0.45781	-0.00003
O	-0.52685	0.73561	0.00002
N	0.84928	0.53514	0.00003
O	1.18312	-0.59911	-0.00002
H	-0.64699	-1.17554	0.00001

cis-HONO

O	1.05824	0.25864	-0.00010
N	0.17185	-0.51952	0.00018
O	-1.08970	0.06636	-0.00017
H	-0.95124	1.03663	0.00090

2_Te (Singlet)

N	-1.03152	1.51254	-0.00006
Te	-1.54297	-0.48076	-0.00011
C	0.30181	1.84697	0.00013
C	1.16969	0.63371	0.00016
C	0.56596	-0.62701	-0.00001
O	0.70321	3.00053	0.00011
H	-1.70564	2.26578	-0.00028
C	2.56365	0.73040	0.00029
C	1.33055	-1.79196	-0.00006
C	3.33579	-0.42402	0.00025
C	2.71874	-1.67993	0.00007
H	0.86658	-2.77171	-0.00018
H	3.32407	-2.57958	0.00004
H	4.41715	-0.35425	0.00035
H	3.00977	1.71849	0.00041

2_Te (Triplet)

N	-0.76346	1.81642	0.00037
Te	-1.63092	-0.39124	-0.00004
C	0.58256	1.91287	-0.00054
C	1.25540	0.56588	-0.00022
C	0.47833	-0.60002	-0.00003
O	1.23034	2.96106	0.00022
H	-1.26733	2.69878	0.00110
C	2.64349	0.46217	-0.00018
C	1.08140	-1.85986	0.00018
C	3.25161	-0.79335	0.00000
C	2.47291	-1.95079	0.00019
H	0.47667	-2.75972	0.00032
H	2.94635	-2.92601	0.00034
H	4.33291	-0.86925	0.00001
H	3.22631	1.37581	-0.00034

2_Te(O)

N	0.73479	1.65527	-0.12343
Te	1.44513	-0.29154	-0.23365
C	-0.61901	1.87127	0.03424
C	-1.39128	0.58546	0.00075
C	-0.68321	-0.60941	-0.10934
O	-1.12021	2.97024	0.16710
H	1.33556	2.46518	-0.02980
C	-2.77992	0.55765	0.11065
C	-1.32801	-1.83867	-0.10850
C	-3.44057	-0.66883	0.10527$_3^-$
C	-2.72061	-1.86018	-0.00082
H	-0.77510	-2.76870	-0.18090
H	-3.24213	-2.81051	0.00535
H	-4.52067	-0.69937	0.18896
H	-3.31627	1.49501	0.20241
O	2.12072	-0.76176	1.41221

2_Te(HOONO)_with_OH

N	2.03376	-1.59701	0.33448
Te	0.09089	-1.34339	-0.30353
C	2.81988	-0.48392	0.50727
C	2.07855	0.76526	0.16466
C	0.74821	0.66710	-0.25277
O	3.97851	-0.52913	0.89251
H	2.44416	-2.49460	0.55302
C	2.68221	2.02236	0.25270
C	0.01175	1.80114	-0.58838
C	1.95795	3.16048	-0.07788
C	0.62789	3.04723	-0.49742
H	-1.01740	1.72251	-0.91629
H	0.06617	3.93751	-0.75801
H	2.42227	4.13751	-0.01324
H	3.71428	2.07421	0.58050
O	-2.68952	-0.34279	-0.05992
O	-3.83771	0.36307	-0.60087
N	-4.74611	0.81129	0.34970
O	-4.46167	0.56050	1.46694
H	-2.84496	-0.31173	0.90990

2_Te(HOONO)_with_N

N	1.76739	-1.86044	0.00005
Te	-0.15747	-1.12894	-0.00006
C	2.81069	-0.96798	0.00002
C	2.32128	0.44185	-0.00009
C	0.94354	0.68048	-0.00011
O	3.98589	-1.30275	0.00001
H	1.99628	-2.84506	0.00009
C	3.20865	1.52103	-0.00015
C	0.43866	1.97971	-0.00018
C	2.71697	2.81985	-0.00022
C	1.33625	3.04511	-0.00023
H	-0.62724	2.17273	-0.00019
H	0.95423	4.06001	-0.00028
H	3.40139	3.66003	-0.00027
H	4.27207	1.31003	-0.00013
N	-3.02795	0.49490	-0.00004
O	-3.32048	1.64372	0.00016
O	-4.09244	-0.38008	0.00025
O	-5.38280	0.23786	0.00069
H	-5.16169	1.19535	0.00067

2_Te(HOONO)_with_H

N	1.31522	-1.86165	0.46955
Te	-0.23975	-1.16151	-0.67834
C	2.31358	-0.98424	0.82669
C	2.07015	0.37894	0.26982
C	0.92577	0.60125	-0.49958
O	3.26789	-1.30372	1.51565
H	1.38063	-2.81370	0.80305
C	2.95691	1.43308	0.50181
C	0.64713	1.85190	-1.04305
C	2.69285	2.68623	-0.03603
C	1.54300	2.89258	-0.80497
H	-0.24405	2.02669	-1.63431
H	1.33992	3.87289	-1.22114
H	3.37726	3.50731	0.14149
H	3.83714	1.24125	1.10473
O	-2.20313	0.70340	1.83573
O	-2.92955	1.07906	0.67676
N	-4.24572	0.39589	0.73861
O	-4.88721	0.72502	-0.16982
H	-1.59067	0.03594	1.46794

2_Te-TS1(O-O activ.)

Te	-0.02096	-1.30190	-0.39323
N	1.85049	-1.67035	0.38923
C	0.76061	0.66320	-0.30885
O	-2.44906	-0.28128	-0.04135
O	-3.75782	0.48952	-0.49844
N	-4.55551	0.87518	0.47753
O	-4.23216	0.61840	1.59439
H	-2.55984	-0.26859	0.93182
C	2.69047	-0.60544	0.61626
C	2.06133	0.68299	0.20052
O	3.80758	-0.71792	1.09538
H	2.17711	-2.58490	0.67099
C	2.73443	1.90110	0.32109
C	0.11912	1.83356	-0.70475
C	2.10683	3.07662	-0.07207
C	0.80478	3.04062	-0.58213
H	-0.89079	1.81303	-1.09490
H	0.31843	3.96052	-0.88707
H	2.62545	4.02400	0.01626
H	3.74105	1.89539	0.72343

2_Te(OH)(ONO)

N	0.60259	-1.98480	-0.18133
Te	-0.85004	-0.51430	-0.37894
C	1.90143	-1.60640	0.05052
C	2.03767	-0.10973	0.05553
C	0.89225	0.67146	-0.10423
O	2.83241	-2.37115	0.21410
H	0.40811	-2.97678	-0.12471
C	3.27098	0.51337	0.22036
C	0.94217	2.06070	-0.11521
C	3.34122	1.90514	0.21571
C	2.18738	2.67174	0.04893
H	0.04246	2.64901	-0.22990
H	2.25014	3.75375	0.05074
H	4.29917	2.39590	0.34298
H	4.15184	-0.10441	0.34913
O	-1.39305	-0.98066	1.46117
O	-1.95393	1.51551	-0.08725
N	-3.22924	1.49545	0.13969
O	-3.69761	0.39621	0.38596
H	-2.30427	-0.66538	1.58691

2_Te(O)(HONO)

N	0.40800	-1.86116	0.02400
Te	-0.27825	-0.35920	-1.20541
C	1.48052	-1.60515	0.86403
C	2.03529	-0.22969	0.64655
C	1.40800	0.59820	-0.28174
O	1.91791	-2.41039	1.65740
H	-0.07761	-2.73988	0.15924
C	3.13264	0.24491	1.36143
C	1.84730	1.89251	-0.52150
C	3.58725	1.54149	1.13061
C	2.94924	2.36118	0.19808
H	1.35080	2.53846	-1.23664
H	3.30565	3.37101	0.03090
H	4.43991	1.91897	1.68262
H	3.60706	-0.40643	2.08622
O	-1.74014	0.42812	-0.39875
O	-4.64158	1.51053	0.82222
N	-4.65304	0.55453	1.52855
O	-3.55670	-0.25209	1.41628
H	-2.91899	0.11248	0.72922

2_Te(OH)

N	-0.35932	1.93191	-0.04715
Te	-1.47219	0.08349	-0.11945
C	0.99925	1.87029	0.09637
C	1.48750	0.45500	0.02346
C	0.54304	-0.57114	-0.06396
O	1.73739	2.83473	0.24659
H	-0.75994	2.85387	0.08884
C	2.84449	0.13991	0.05799
C	0.93120	-1.90588	-0.14433
C	3.24455	-1.19241	-0.01294
C	2.29258	-2.20934	-0.11508
H	0.18921	-2.69050	-0.22893
H	2.60980	-3.24419	-0.17690
H	4.29921	-1.44140	0.00791
H	3.56215	0.94791	0.13903
O	-2.13627	-1.78992	0.54653
H	-1.69600	-2.16786	1.31725

Table 4S. B3LYP/BS1 calculated energetics (in a.u.) of all structures reported in the paper.

Structures	E_{tot}	E_{tot}+ZPC	Enthalpy	G
NO_2	-205.140697	-205.131906	-205.128030	-205.155260
***cis*-HOONO**	-280.919107	-280.896022	-280.890883	-280.922266
***cis*-HONO**	-205.769980	-205.749919	-205.745805	-205.773903
OH	-75.754884	-75.746559	-75.743254	-75.763491
2_Te	-407.916886	-407.812429	-407.803068	-407.847618
2_Te(O)	-483.105096	-482.997623	-482.987073	-483.034158
2_Te + *cis*-HOONO	-688.835993	-688.708451	-688.693951	-688.769884
2_Te(HOONO)_with_OH	-688.848091	-688.719779	-688.704197	-688.767140
2_Te(HOONO)_with_N	-688.845361	-688.716892	-688.701184	-688.765012
2_Te(HOONO)_with_H	-688.844436	-688.716347	-688.702150	-688.760160
2_Te-TS1(O-O activ.)	-688.846884	-688.719511	-688.704551	-688.764500
2_Te(OH)(NO_2)	-688.919487	-688.789485	-688.774911	-688.831229
2_Te(OH)	-483.738063	-483.620314	-483.609090	-483.657750
2_Te(O)(HONO)	-688.893349	-688.764530	-688.750085	-688.809366
2_Te(OH) + NO_2	-688.878760	-688.752220	-688.737120	-688.813010
2_Te(O) + *cis*-HONO	-688.875076	-688.747542	-688.732878	-688.808061