

Supporting Information

Stability, electronic properties, and decomposition mechanisms of 2,6-diamino-3,5-dinitropyrazine-1-oxide crystals with different vacancy defects

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Table S1 Absolute energies of all the structures.

Model	V0	V1	V2-1	V2-2	V2-3
E(eV)	-51068.72	-50003.55	-48938.63	-48938.40	-48938.37
Model	V2-4	V3-1	V3-2	V3-3	V3-4
E(eV)	-48938.59	47873.53	-47873.77	-47873.60	-47873.35

Cartesian coordinates of all the optimized geometries

V0

N	4.27233319	2.62726926	0.86511389
C	-0.02707431	2.84274647	24.02600670
C	-1.19163736	2.28145001	23.41138082
N	-2.04095172	1.54985302	24.21293232
C	2.23597837	1.32298218	1.09481527
C	3.44681857	1.88580650	1.61981439
N	3.91964095	1.63381878	2.96151692
O	3.27279282	0.87159927	3.69777734
O	4.98583148	2.14850645	3.30724011
N	0.94061005	3.61622028	23.28499298
O	0.95325898	3.56057774	22.05333856
O	1.74238342	4.31363491	23.92151856
N	1.34281390	0.56417659	1.76707831
H	0.51863987	0.20771604	1.24932078
H	1.45914576	0.34525895	2.76836389
N	-1.53931863	2.38151776	22.11140840
H	-2.43430353	1.96589466	21.80956009
H	-0.95849119	2.90103405	21.42715747
O	-3.09347922	0.99389079	23.66878472
N	3.51102467	10.73305829	3.20927214
C	3.80967666	10.93614291	4.50069304
C	4.97530448	10.37695221	5.11530471
N	5.82482403	9.64493641	4.31420536
C	5.54864711	9.43055860	2.98011179
C	4.33698220	9.99178592	2.45511801
N	3.86450600	9.73778916	1.11366372
O	4.50957503	8.97256347	0.37946630
O	2.79905469	10.25399353	0.76626830
N	2.84150471	11.70905870	5.24119402
O	2.83422148	11.66106982	6.47311301
O	2.03370351	12.39862465	4.60369632
N	6.44218198	8.67198412	2.30815011
H	7.26733640	8.31762870	2.82581696
H	6.32634404	8.45277345	1.30695375
N	5.32354196	10.47878483	6.41492008
H	6.21979752	10.06570154	6.71660003
H	4.74343256	10.99986697	7.09871466
O	6.87797508	9.09039747	4.85858635
N	0.02581391	13.59000898	7.28551095
C	0.32405244	13.38860239	8.57712102
C	1.48866451	13.94977297	9.19176881

N	2.33803561	14.68138626	8.39025410
C	2.06221433	14.89426790	7.05589154
C	0.85133988	14.33152162	6.53091862
N	0.37860991	14.58348734	5.18918629
O	1.02516954	15.34611893	4.45307790
O	-0.68721718	14.06821562	4.84310477
N	-0.64359652	12.61509941	9.31808106
O	-0.65554103	12.66963181	10.54977246
O	-1.44616580	11.91860250	8.68139893
N	2.95537535	15.65310376	6.38366082
H	3.77956421	16.00952763	6.90142083
H	2.83900726	15.87216074	5.38241365
N	1.83635200	13.84959630	10.49173821
H	2.73138558	14.26513227	10.79358597
H	1.25545468	13.33008255	11.17594765
O	3.39068006	15.23715120	8.93437115
N	0.78712525	5.48419543	4.94170468
C	0.48844348	5.28104451	3.65030051
C	21.86328635	5.84017200	3.03570680
N	21.01372401	6.57221016	3.83678339
C	21.29002484	6.78674776	5.17085861
C	-0.03878471	6.22556553	5.69582228
N	0.43379337	6.47950776	7.03725663
O	-0.21097376	7.24535222	7.77126980
O	1.49874664	5.96268292	7.38494528
N	1.45668462	4.50807706	2.90994742
O	1.46359219	4.55559123	1.67791826
O	2.26475366	3.81910306	3.54747055
N	20.39653270	7.54539897	5.84278047
H	19.57127024	7.89957956	5.32517552
H	20.51234597	7.76468886	6.84397028
N	21.51507061	5.73826360	1.73607992
H	20.61895446	6.15150904	1.43428333
H	22.09527742	5.21724751	1.05231671
O	19.96052669	7.12663840	3.29240877
N	9.90752713	2.62731630	0.86511793
C	5.60810805	2.84281416	24.02599857
C	4.44355609	2.28147804	23.41138348
N	3.59426194	1.54986140	24.21294396
C	7.87122528	1.32291824	1.09483369
C	9.08207324	1.88576629	1.61981033
N	9.55504199	1.63374343	2.96143656
O	8.90841210	0.87117417	3.69761351
O	10.62100481	2.14877860	3.30724932

N	6.57579782	3.61620892	23.28497808
O	6.58862864	3.56033804	22.05341536
O	7.37737289	4.31390469	23.92154377
N	6.97814607	0.56404088	1.76706738
H	6.15381961	0.20779410	1.24940557
H	7.09438925	0.34517104	2.76835654
N	4.09591175	2.38155873	22.11140024
H	3.20114628	1.96559365	21.80938137
H	4.67682749	2.90099703	21.42717787
O	2.54173789	0.99381142	23.66876807
N	9.14621004	10.73306914	3.20911879
C	9.44485830	10.93621007	4.50053785
C	10.61055578	10.37713604	5.11516048
N	11.46012187	9.64511766	4.31409064
C	11.18391222	9.43065679	2.98002039
C	9.97222143	9.99182324	2.45500646
N	9.49991774	9.73784068	1.11347679
O	10.14494855	8.97257107	0.37935710
O	8.43449168	10.25427317	0.76596726
N	8.47671192	11.70921347	5.24096185
O	8.47007177	11.66211010	6.47299216
O	7.66821203	12.39790732	4.60338143
N	12.07747914	8.67211017	2.30804835
H	12.90253592	8.31763183	2.82579525
H	11.96156426	8.45277113	1.30690093
N	10.95883007	10.47902936	6.41476497
H	11.85527964	10.06624893	6.71631580
H	10.37873968	11.00017398	7.09854170
O	12.51336681	9.09075554	4.85844214
N	5.66088034	13.58996142	7.28550724
C	5.95913524	13.38852673	8.57710850
C	7.12371559	13.94973924	9.19176003
N	7.97306910	14.68137492	8.39024765
C	7.69721674	14.89432507	7.05588862
C	6.48632939	14.33155606	6.53092322
N	6.01353777	14.58363142	5.18924017
O	6.65978101	15.34655555	4.45327712
O	4.94785944	14.06796990	4.84307073
N	4.99145441	12.61510183	9.31809607
O	4.97929179	12.66989818	10.54967035
O	4.18909284	11.91838264	8.68135376
N	8.59031055	15.65324594	6.38369041
H	9.41466244	16.00945952	6.90136306
H	8.47403375	15.87226562	5.38242345

N	7.47135230	13.84954582	10.49173098
H	8.36615103	14.26542658	10.79376580
H	6.89037240	13.33011389	11.17591933
O	9.02569438	15.23723344	8.93441380
N	6.42217943	5.48420462	4.94183488
C	6.12351138	5.28099117	3.65041881
C	4.95778817	5.84000808	3.03583508
N	4.10816970	6.57203945	3.83687415
C	4.38450798	6.78665353	5.17092773
C	5.59620859	6.22554775	5.69590687
N	6.06873561	6.47939780	7.03743836
O	5.42386343	7.24536159	7.77138798
O	7.13352097	5.96239627	7.38520638
N	7.09174209	4.50793328	2.91016822
O	7.09795299	4.55452006	1.67800884
O	7.90046935	3.81980829	3.54779278
N	3.49097708	7.54526128	5.84286071
H	2.66583104	7.89955785	5.32519000
H	3.60687039	7.76468140	6.84400539
N	4.60954375	5.73803436	1.73621104
H	3.71324110	6.15095656	1.43453828
H	5.18973507	5.21695508	1.05247959
O	3.05489243	7.12626285	3.29256755
N	15.54262437	2.62737457	0.86533950
C	11.24318284	2.84297553	24.02624998
C	10.07859322	2.28177048	23.41160016
N	9.22923330	1.55012804	24.21311555
C	13.50628886	1.32300464	1.09496933
C	14.71717647	1.88577547	1.61994641
N	15.18996306	1.63369599	2.96161079
O	14.54372207	0.87076512	3.69756562
O	16.25566499	2.14937656	3.30779113
N	12.21087630	3.61642731	23.28532471
O	12.22303358	3.56160400	22.05368998
O	13.01321876	4.31311197	23.92200883
N	12.61319595	0.56408063	1.76717002
H	11.78884315	0.20786771	1.24949183
H	12.72947855	0.34506506	2.76842821
N	9.73094739	2.38195761	22.11162506
H	8.83614879	1.96607538	21.80959207
H	10.31192932	2.90139641	21.42743538
O	8.17660666	0.99427174	23.66892905
N	14.78131729	10.73313611	3.20897974
C	15.07998507	10.93635420	4.50041937

C	16.24571633	10.37733719	5.11501130
N	17.09532445	9.64530127	4.31397141
C	16.81900381	9.43067209	2.97990831
C	15.60729118	9.99178984	2.45493010
N	15.13480230	9.73789902	1.11340480
O	15.77962487	8.97196086	0.37945864
O	14.06996615	10.25493548	0.76564734
N	14.11181165	11.70938153	5.24069911
O	14.10557581	11.66282856	6.47280918
O	13.30298252	12.39755045	4.60305898
N	17.71251515	8.67206022	2.30797665
H	18.53766553	8.31776162	2.82565141
H	17.59663043	8.45264741	1.30685230
N	16.59396345	10.47930699	6.41463688
H	17.49028482	10.06637202	6.71631063
H	16.01375749	11.00039825	7.09836019
O	18.14862741	9.09104422	4.85828185
N	11.29596772	13.59001951	7.28571307
C	11.59420581	13.38868408	8.57733297
C	12.75874482	13.95001767	9.19196719
N	13.60803373	14.68163276	8.39041140
C	13.33228090	14.89441319	7.05601913
C	12.12142345	14.33156255	6.53103902
N	11.64856229	14.58366678	5.18940271
O	12.29508321	15.34615209	4.45324513
O	10.58249640	14.06858002	4.84358245
N	10.62652829	12.61531551	9.31842752
O	10.61367199	12.67115848	10.54991336
O	9.82492477	11.91761299	8.68179113
N	14.22535976	15.65329508	6.38378424
H	15.04970160	16.00954468	6.90145598
H	14.10912869	15.87217145	5.38249212
N	13.10638247	13.84992814	10.49193501
H	14.00115591	14.26589889	10.79395455
H	12.52547630	13.33049528	11.17616923
O	14.66056533	15.23769502	8.93460261
N	12.05728872	5.48424773	4.94169807
C	11.75864381	5.28113097	3.65027236
C	10.59293253	5.84020684	3.03567567
N	9.74336864	6.57222061	3.83675863
C	10.01959580	6.78666788	5.17082846
C	11.23126932	6.22550179	5.69582928
N	11.70369897	6.47937672	7.03734999
O	11.05854187	7.24475115	7.77150603

O	12.76901439	5.96301190	7.38484934
N	12.72682304	4.50808962	2.90992564
O	12.73343369	4.55527478	1.67779550
O	13.53525759	3.81940988	3.54743115
N	9.12603628	7.54520922	5.84280672
H	8.30099758	7.89968300	5.32507022
H	9.24196461	7.76454372	6.84396037
N	10.24465229	5.73832140	1.73606165
H	9.34822263	6.15110331	1.43452269
H	10.82474473	5.21719053	1.05229266
O	8.69014515	7.12656207	3.29243404
N	21.17768543	2.62731508	0.86533321
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C	15.71365480	2.28173168	23.41159635
N	14.86427260	1.55011382	24.21310523
C	19.14129363	1.32306292	1.09495308
C	20.35217456	1.88580811	1.61995107
N	20.82479616	1.63375754	2.96168332
O	20.17833967	0.87121272	3.69774111
O	21.89073714	2.14910274	3.30779375
N	17.84593021	3.61641257	23.28531115
O	17.85789252	3.56188040	22.05361706
O	18.64845028	4.31287995	23.92198719
N	18.24811197	0.56422074	1.76718431
H	17.42390880	0.20779271	1.24941038
H	18.36448010	0.34515822	2.76843844
N	15.36596748	2.38190903	22.11163539
H	14.47093730	1.96638212	21.80977870
H	15.94685179	2.90142955	21.42741671
O	13.81162887	0.99435593	23.66894916
N	20.41638735	10.73313716	3.20913375
C	20.71505469	10.93629581	4.50058010
C	-0.65977125	10.37716177	5.11515790
N	0.18978545	9.64512490	4.31408864
C	-0.08650186	9.43058010	2.98000212
C	21.24230381	9.99176138	2.45504299
N	20.76963951	9.73786024	1.11358645
O	21.41449408	8.97195713	0.37957354
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N	19.74684703	11.70925304	5.24090923
O	19.73996391	11.66175659	6.47294011
O	18.93870829	12.39825862	4.60338750
N	0.80697161	8.67193497	2.30808036
H	1.63221635	8.31775520	2.82567372

H	0.69116307	8.45264954	1.30690956
N	-0.31156054	10.47906788	6.41479785
H	0.58456099	10.06582434	6.71660102
H	-0.89179355	11.00009608	7.09853724
O	1.24298812	9.09068126	4.85842834
N	16.93115301	13.59006061	7.28570789
C	17.22937415	13.38875420	8.57733995
C	18.39393994	13.95004855	9.19197267
N	19.24324733	14.68164513	8.39041864
C	18.96752753	14.89435792	7.05602241
C	17.75668438	14.33152715	6.53103038
N	17.28389023	14.58353342	5.18934213
O	17.93071017	15.34573673	4.45305632
O	16.21767156	14.06882757	4.84361264
N	16.26171737	12.61529956	9.31838942
O	16.24906248	12.67092574	10.55001411
O	15.45991448	11.91783915	8.68183294
N	19.86067230	15.65316036	6.38375958
H	20.68484966	16.00961799	6.90152073
H	19.74435252	15.87207650	5.38248941
N	18.74162047	13.84997719	10.49194084
H	19.63661994	14.26561241	10.79378112
H	18.16079058	13.33046340	11.17619503
O	20.29578704	15.23762063	8.93456751
N	17.69249489	5.48426248	4.94156601
C	17.39383713	5.28120101	3.65015564
C	16.22819920	5.84038402	3.03554687
N	15.37868143	6.57239491	3.83666369
C	15.65486699	6.78677101	5.17075421
C	16.86652747	6.22553556	5.69574240
N	17.33900242	6.47951624	7.03717457
O	16.69393111	7.24474203	7.77139313
O	18.40447827	5.96329694	7.38459644
N	18.36202766	4.50827151	2.90967581
O	18.36931298	4.55631525	1.67771432
O	19.16976829	3.81869143	3.54713110
N	14.76133845	7.54534419	5.84272293
H	13.93618339	7.89969589	5.32505012
H	14.87718472	7.76455177	6.84392014
N	15.87995072	5.73855336	1.73593187
H	14.98369626	6.15164071	1.43426620
H	16.46005321	5.21748365	1.05213570
O	14.32552433	7.12692199	3.29227354
N	2.93860644	2.63197828	9.01600765

C	2.64039532	2.83331278	7.72437441
C	1.47584048	2.27200733	7.10973752
N	0.62653651	1.54042091	7.91129241
C	0.90224875	1.32769849	9.24569247
C	2.11311130	1.89053150	9.77065859
N	2.58584857	1.63848786	11.11235309
O	1.93910732	0.87637748	11.84860677
O	3.65207625	2.15319812	11.45809360
N	3.60800748	3.60673303	6.98320320
O	3.62067334	3.55115700	5.75170163
O	4.40987300	4.30427343	7.61986526
N	0.00909838	0.56890610	9.91793845
H	-0.81508316	0.21244388	9.40018242
H	0.12541514	0.34999091	10.91918526
N	1.12814896	2.37207881	5.80974899
H	0.23311808	1.95643993	5.50791440
H	1.70899682	2.89159859	5.12547883
O	-0.42604162	0.98443190	7.36714493
N	2.17732141	10.73779384	11.36017394
C	2.47594065	10.94084670	12.65157648
C	3.64158620	10.38167114	13.26616898
N	4.49110780	9.64965476	12.46506209
C	4.21491656	9.43529420	11.13096597
C	3.00326812	9.99652488	10.60596486
N	2.53073091	9.74258126	9.26451786
O	3.17584633	8.97731387	8.53031259
O	1.46530342	10.25877626	8.91712988
N	1.50772155	11.71381434	13.39193578
O	1.50045547	11.66578487	14.62397251
O	0.69998999	12.40328380	12.75459226
N	5.10845176	8.67671846	10.45898986
H	5.93359207	8.32236581	10.97664437
H	4.99260020	8.45751200	9.45778344
N	3.98983367	10.48349096	14.56578233
H	4.88605396	10.07042130	14.86746959
H	3.40973259	11.00456880	15.24956580
O	5.54422303	9.09514649	13.00943302
N	-1.30788715	13.59473890	15.43634416
C	-1.00969683	13.39331735	16.72794272
C	0.15491753	13.95448331	17.34258718
N	1.00429959	14.68609950	16.54108325
C	0.72848241	14.89898795	15.20670371
C	-0.48240440	14.33622817	14.68173146
N	-0.95506020	14.58826362	13.33999870

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V2-1

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V3-2

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O	15.40279928	15.55429426	20.58673407
O	13.53517439	14.49746559	20.92043996
N	17.33042326	12.74127427	0.95844654
O	17.42283616	12.51798340	2.17249315
O	16.38817233	12.32580410	0.27661591
N	17.19896908	15.80436691	22.60272341
H	18.00709383	16.16112094	23.14651702
H	17.07076788	16.06013535	21.61471400
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H	20.67520787	14.34293962	2.62535691

H	19.20582977	13.36397027	2.93640202
O	21.40031727	15.35915988	0.84633403
N	15.02794072	5.59848787	21.16579576
C	14.72982961	5.39162880	19.87605812
C	13.55767563	5.94092952	19.26278376
N	12.70241154	6.67093322	20.05988709
C	12.99554652	6.91633642	21.38593932
C	14.20291190	6.34913034	21.91611528
N	14.66238191	6.57145226	23.26331598
O	13.99069766	7.27814346	24.03144680
O	15.75379007	6.08937087	23.59034763
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O	15.68086314	4.59906818	17.91691491
O	16.55658866	3.99458225	19.80565869
N	12.11145772	7.68746378	22.05243377
H	11.30429767	8.06525413	21.52524012
H	12.24540812	7.93986713	23.04274258
N	13.19397520	5.80667039	17.97133246
H	12.30203468	6.22827408	17.67129639
H	13.78078926	5.29891322	17.28351538
O	11.61100713	7.15898976	19.53152762